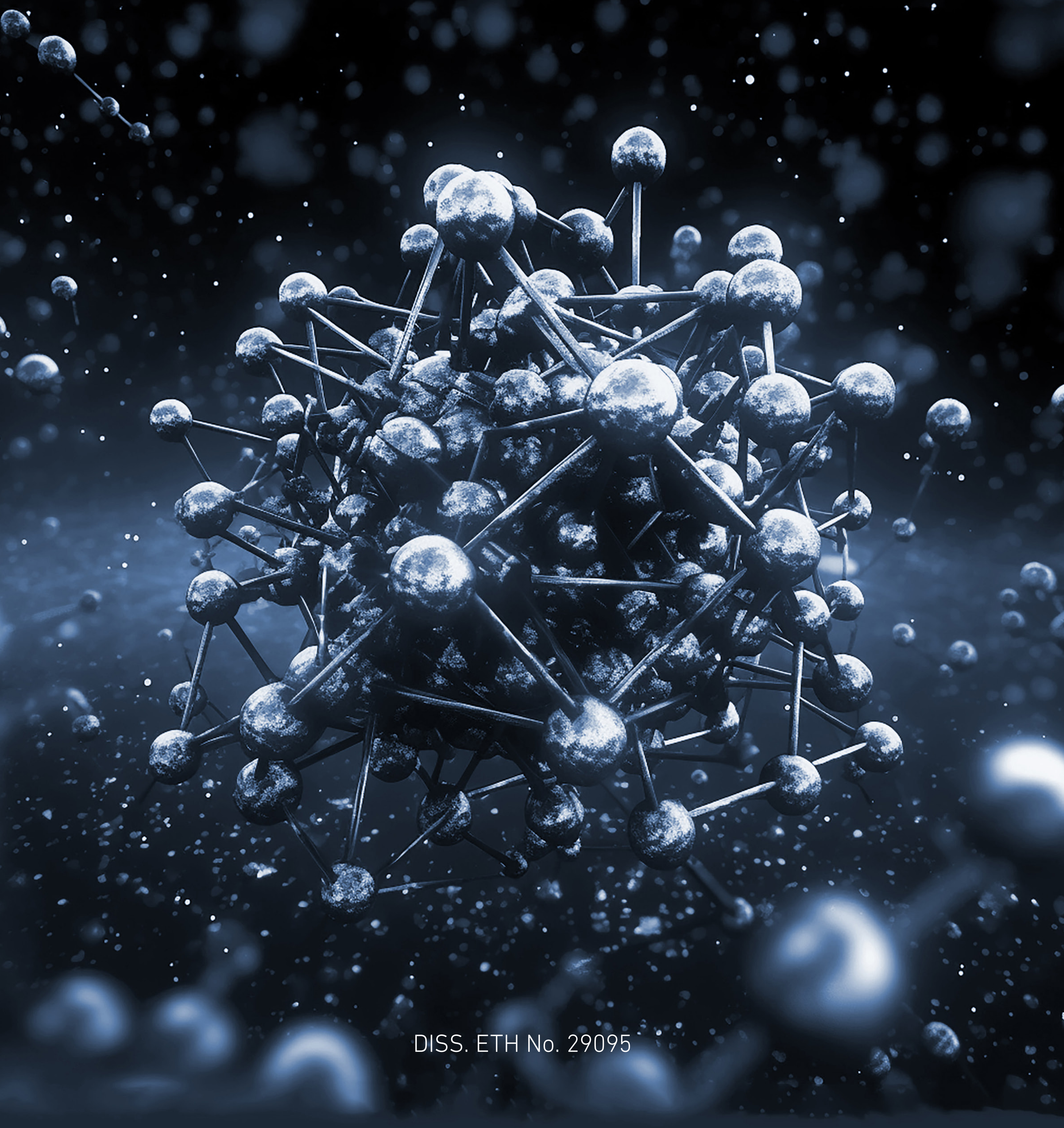
Diagnosing and Promoting the Understanding of Chemical Bonding

Adrian Zwyssig



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Diagnosing and Promoting the Understanding of Chemical Bonding

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ADRIAN ZWYSSIG

MSc ETH Chemistry, ETH Zurich
Born on 14.03.1989

Supervisor: Prof. Dr. Elsbeth Stern
Co-Supervisor: Prof. em. Dr. Antonio Togni
Co-Referee: Prof. Dr. Ilka Parchmann

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Abstract

Understanding the forces and chemical bonds that hold together substances is as challenging as it is fundamental for students' comprehension of more advanced concepts in chemistry. What mainly impedes students' learning about chemical bonding is overgeneralization: Typically, students neglect the differences between covalent, ionic, and metallic bonds and apply the model of covalent bonding to all bonding situations. This overgeneralization was confirmed by our assessment of university science undergraduates' knowledge before attending lectures. 40 % of these students (N = 1946) wrongfully assumed the existence of molecules in sodium chloride, an ionic compound. The assessment further revealed the prevalence of uncertainties concerning the differences between chemical bonds and intermolecular forces. Thus, to foster students' ability to keep the differences between these similar concepts in mind, we designed teaching materials containing multiple comparing and contrasting activities (23 lessons), introducing the three types of chemical bonds simultaneously. In a pre- and post-test classroom intervention study at Swiss Gymnasiums (N = 326, grade 10) the materials' effectiveness was evaluated. Comparing and contrasting activities fostered students' conceptual understanding more strongly ($d = 1.05$, $CI_{95}[0.78; 1.31]$) and were better suited to promote conceptual change than the regular sequential introduction of the different bonding types. Additionally, the same teaching materials were used in a seven-lesson university preparatory course (N = 296). Science students' conceptual understanding increased strongly ($d = 2.44$, $CI_{95}[2.21; 2.66]$), and the frequency of misconceptions was reduced drastically from pre- to post-test ($0.81 < d < 2.24$). This study will help inform chemistry educators about students' main challenges when learning about chemical bonds and provides a more effective and classroom-evaluated approach how to teach chemical bonding with increased and sustainable learning gains.

Zusammenfassung

Zu verstehen, was Atome in Stoffen zusammenhält, ist für viele Schülerinnen und Schüler eine grosse Herausforderung. Ein vertieftes Verständnis der chemischen Bindung und der zwischenmolekularen Kräfte bildet jedoch die Grundlage, um im Chemieunterricht komplexere Themen behandeln zu können. Das grösste Hindernis stellt dabei die Tendenz zur Übergeneralisierung dar: Typischerweise vernachlässigen Lernende die Unterschiede zwischen kovalenten, ionischen und metallischen Bindungen und wenden das Modell der kovalenten Bindung auf alle Bindungssituationen an. Diese Tendenz zur Übergeneralisierung konnte durch die Untersuchung des Verständnisses angehender Naturwissenschaftsstudierender (N = 1946) vor dem Besuch von Universitätsvorlesungen bestätigt werden. 40 % der Studierenden nahmen beispielsweise fälschlicherweise an, dass Natriumchlorid (eigentlich eine ionische Verbindung) aus Molekülen aufgebaut ist. Die Untersuchung zeigte zudem, dass auch nach dem Unterricht zu chemischen Bindungen auf der Gymnasialstufe weiterhin Unsicherheiten beim Unterscheiden von chemischen Bindungen und zwischenmolekularen Kräften weit verbreitet sind.

Um die Fähigkeit der Lernenden zu fördern, die Bindungsarten besser auseinander zu halten, haben wir deshalb eine Unterrichtseinheit von 23 Lektionen entwickelt, die viele vergleichende und kontrastierende Aufgaben enthält. Im Unterschied zu herkömmlichen Lernmaterialien werden die Bindungsarten bei diesem Ansatz bereits am Anfang gleichzeitig eingeführt. Zudem werden bei der Behandlung der einzelnen Bindungsarten stets die Unterschiede zu den anderen Bindungsarten hervorgehoben.

In einer quasi-experimentellen Vergleichsstudie an Schweizer Gymnasien (N = 326, 10. Klassenstufe) wurde die Lernwirksamkeit dieser Unterrichtsmaterialien untersucht. Dabei zeigte sich, dass im Vergleich zur herkömmlichen sequentiellen Behandlung der Bindungsarten das vermehrte Vergleichen und Kontrastieren die Schülerinnen und Schüler stärker beim Aufbau von konzeptuellem Verständnis unterstützt ($d = 1.05$, $CI_{95}[0.78; 1.31]$). Zusätzlich wurden die Lernmaterialien in einem kurzen Repetitionskurs für angehende Naturwissenschaftsstudierende eingesetzt (N = 296). Während sich das konzeptuelle Verständnis der Studierenden nach den sieben Lektionen stark verbesserte ($d = 2.44$, $CI_{95}[2.21; 2.66]$), konnte die Häufigkeit von Fehlkonzepten im Vergleich zum Vortest deutlich reduziert werden ($0.81 < d < 2.24$). Mit diesen Materialien wird Lehrpersonen daher ein Ansatz zur Verfügung gestellt, mit dem sie chemische Bindungen und zwischenmolekulare Kräfte lernwirksam und nachhaltig unterrichten können.

1 The Significance and Challenges of Understanding Chemical Bonding

Chemistry evolves around the central theme of the smallest particles. To make sense of the different macroscopic properties of substances, students also need to understand how the smallest particles (i.e. atoms, ions, or molecules) interact with each other. Since students can never actually see those smallest particles and their interactions, the understanding of those topics is prone to misconceptions.

Inherent Challenges Associated with the Nature of Smallest Particles

Some difficulties associated with those fundamental concepts are inherent to chemistry. The term "smallest particles" is ambiguous, since it is used to describe different entities depending on the level of description. If we look at a glass of water on our table for example and ask ourselves what the smallest particle of water might be, we might come to the conclusion that it must be one water molecule. While this is certainly true on a certain level of description, water molecules are comprised of one oxygen atom and two hydrogen atoms. And if we go deeper into one of those atoms, we even find that the atoms themselves consist of protons, neutrons, and electrons, which again consist of quarks being the actual smallest building block scientists are currently aware of. Nevertheless, the term particle is used in all of those cases, making it even harder for students to build up a concise mental framework of the particle world of substances.

While chemistry experts are used to fluently switching between the different levels, this transition remains a challenge for many novices and laypersons. However, for students to make sense of fundamental concepts in chemistry the interaction between those particles is essential. Without an understanding of such concepts, students will have difficulties explaining substances' properties and even the matter humans themselves are comprised of.

The understanding of the constitution and nature of the elemental building blocks of atoms, electrons, protons, and neutrons falls into the scope of nuclear physicists. Chemists and chemistry instructors on the other hand focus on how atoms of different elements are built up with such building blocks and investigate the interaction between atoms. What are the mechanisms that hold the small entities (i.e. atoms, molecules, and ions) together to make up observable matter? If we succeed in teaching students appropriate concepts to understand the interaction between those smallest particles, they can rationalize and even predict the properties and behavior of compounds on a macroscopically observable level even though they have never seen an atom itself.

Multiple Possibilities for Atoms to Hold Together

Unfortunately, predicting chemical behavior is no easy feat due to another inherent challenge: There is more than one possible interaction of how atoms are held together. While every student has at least once observed that water boils at 100 °C (under atmospheric pressure), it isn't an easy task to predict what water looks like in the gaseous state. In fact to make correct predictions students need to know that there are two different kinds of interactions present in water (Figure 1). There are so-called covalent bonds (in blue) and hydrogen bonds (green dashed) present in liquid water. Students need an understanding of the differences between those kinds of interactions since the superficial properties are similar – in both cases the hydrogen atom is connected to an oxygen atom. One of the main differences lies in the strength of the bonds. While the hydrogen bonds (blue in Figure 1) break at 100 °C (at atmospheric pressure) and water is vaporized, i.e. the water is present as separate water molecules in a gaseous state, the temperature needs to rise above 2000 °C to break the covalent bonds (red in Figure 1) and thereby separating oxygen and hydrogen atoms (Funk, 2001).

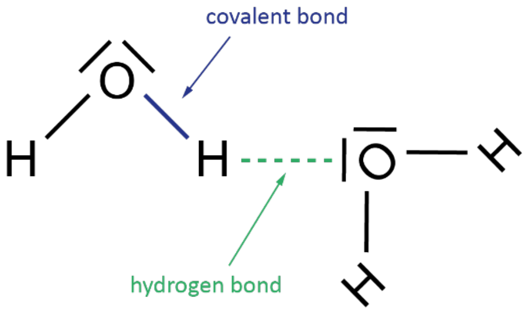

Figure 1: Hydrogen bond (green dashed) and covalent bond (blue) of a hydrogen atom of a water molecule.

This means that water molecules do not dissociate into single hydrogen and oxygen atoms when water is heated up to 100 °C, but stay intact as single water molecules. Due to the vast differences in strength and the practical implications, chemists distinguish between strong chemical bonds, such as covalent bonds, and much weaker intermolecular forces, like for example hydrogen bonds.

Similar Surface Characteristics - Different Bonding Situation

Given students have understood the differences of bonds in water, they might tend to overgeneralize, as there are two more possibilities of how atoms can combine to constitute substances: ionic or metallic bonding.

When chemistry novices see a table salt crystal and compare what they see to a known thing like an ice cube of water, they recognize the many similarities like transparency and the way it breaks upon application of pressure (see Figure 2). Therefore, they might be inclined to transfer what they know about water to the new substance. Upon being told that table salt has the chemical formula NaCl, they might easily be persuaded to think of table salt as being comprised of small NaCl molecules holding together similarly as water molecules do. Experts on the other hand know about the different kinds of chemical bonds present in this substance and avoid focusing on the surface characteristics.

Figure 2: Water ice cubes (left) and sodium chloride crystal (right) with similar surface characteristics.

It is possible to analyze the distances between the atoms in a crystal structure using x-ray diffraction. Such analysis allows the estimation of the distances between atoms. The distance itself is a measure of the strength of an attraction, i.e. the closer the stronger the attracting force, usually. Considering the weaker nature of intermolecular forces we should be able to find water molecules with one oxygen and two hydrogen atoms in close proximity (Figure 3, left). While this is the case for water, we cannot observe pairs in a sodium chloride crystal (Figure 3, right).

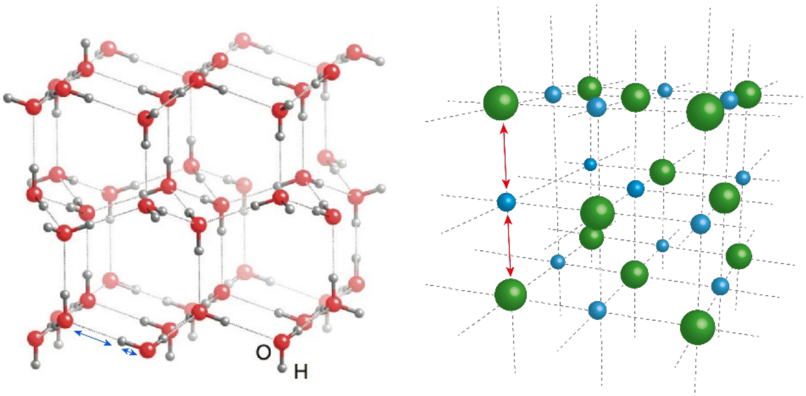

Figure 3: Left; Solid ice crystal (Nick Greeves, n.d., arrows added) with highlighted distance differences (blue arrows) and Sodium chloride crystal structure (right) with highlighted equal distances (red arrows) between a sodium ion (blue) and two neighboring chloride ions (green).

But while some characteristics are similar, others are quite different: Solid ice melts above 0 °C and boils at 100 °C (under atmospheric pressure). Are you able to predict the melting temperature of table salt? Is it even possible to melt a solid sodium chloride crystal? The answer is yes, but we need to heat table salt to over 800 °C to melt a sodium chloride crystal and up to 1500 °C to obtain gaseous sodium chloride. This means particles in sodium chloride must exhibit stronger attracting forces since more energy must be invested to obtain single sodium chloride particles in the gas phase. But what is the reason for this?

The answer is quite simple: Even though both substances form transparent crystals, the way those substances are built up differs strongly: The building blocks of table salt are charged atoms, so-called ions, i.e. positively charged sodium cations (Figure 3, right, light blue) and negatively charged chloride anions (Figure 3, right, green). The attraction between the opposite charges is the reason why sodium chloride is formed and held together in the shown regular manner (Figure 3, right). Such an arrangement and attraction of ions is typical for ionic bonding. Ionic bonding is similar in strength to covalent bonds but there are no weaker intermolecular forces present in table salt. To obtain liquid or gaseous sodium chloride, it is, therefore, necessary to weaken or break up the strong ionic bonds – explaining the high melting and boiling temperature of table salt.

Mode of Representation

Another inherent difficulty is associated with the above-mentioned impossibility to observe atoms or ions by eye. Since we cannot see atoms, ions, or small molecules, we need methods of how to represent them. While Figure 3 might illustrate the fact that there are no NaCl molecules or subunits present in a sodium chloride crystal, it might also give rise to a variety of misconceptions. The shown colored spheres do not differ from the atoms in water shown to its left. Students might also mistake the dashed lines, meant to illustrate the symmetrical alignment of the ions, for covalent bonds. Chemistry educators of course know about such difficulties and try to represent different bonding situations differently but the adequate illustration of bonding situations remains an inherent challenge when learning about the chemical bond.

Ambiguities in the Use of Chemical Language

Even before students are instructed on chemical bonding, they usually have an understanding of terms like *atom*, *molecule*, *substance,* or *matter*. Additional terms like *ionic* and *metallic lattice* have to be implemented into students' mental concepts of the particle world. While students' definitions of certain terms like *molecule* are typically broad, the chemistry experts' definition is more refined. It is a general challenge to sharpen students' definitions of terms students have already encountered before instruction of the concepts involved. The term *Lattice*[1] for example is used in daily life as well. This is a potential opening for the undesired transfer of characteristics of daily life's meaning onto the term being used in the context of chemical bonding models.

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[1] This is particularly true in German where the term "Gitter" is more commonly used to define macroscopic objects.

Additionally, depending on the language spoken and the chemistry field the term *molecule* is not as sharply defined as one would expect: A *molecule* is narrowly defined as a neutral ensemble of two and more non-metallic atoms held together by covalent bonds. This strict definition is helpful when trying to keep molecules and molecular substances apart from ions and ionic compounds. Unfortunately, even some experts in the field of organic chemistry and quantum mechanics or biochemistry will sometimes use the term molecule for some ionic entities (e.g. polyatomic ions) or even single atoms (in the case of noble gases for example). The *International Union of Pure and Applied Chemistry* (IUPAC) clearly defines a molecule as being neutral (Muller, 1994). Unfortunately, this does not prevent some chemistry textbooks from making use of the unspecific definition of the term molecule. This problem is more pronounced in English-speaking parts of the world. This might of course be a further source of confusion for students. In German-speaking parts of the world, the term molecule is generally not used for ions. Maybe influenced by the term's use in the English-speaking science community we find the broader definition of the term also in the World Wide Web: Wikipedia's German site for the term *molecule* for example introduces a molecule as a particle constituted by more than two atoms which are held together by chemical bonds ("Molekül", 2022, para. 1) . A specification about the nature of the bond or the condition of electrical neutrality is not given in this definition. Even though the more strict definition is given in the following paragraph one can see the difficulty chemistry educators face: Different sources of information outside the classroom define terms differently.

Quantum Mechanics as the Fundamental Theory to Explain Chemical Bonds

Understanding the nature of a chemical bond is complex. What is the reason for two atoms to hold together? The answer to this seemingly simple question is everything but trivial: Even chemistry experts will have a hard time fundamentally *explaining* why that is the case.

Quantum mechanics is the most fundamental theory to describe chemical and physical phenomena on the microscopic level. If we were to compare chemistry to other subjects, like learning about a language, the theory would be as fundamental as knowing how to interpret the letters of a word. But why don't we teach students the most fundamental theory of all from the very beginning? The answer is very simple: We must acknowledge that quantum mechanics is highly complex and parts of it are highly counter-intuitive. Of course, that is, illogical seen only from the standpoint of classical mechanics. The problem is, that the way we think and represent concepts in our minds is of course highly dependent on everything we have so far experienced, seen, and observed. And most of that is, in fact, something stemming from the macroscopic realm, i.e. phenomena that can be explained with classical mechanics. The realm of the microscopic world, i.e. the quantum realm, is behaving according to other rules. While quantum mechanics is not taught as an introduction to chemistry novices, it is of course an integral part of the education of chemists. Chemistry students at university will learn how to use the theory of quantum mechanics to describe quantum phenomena, like for example the behavior of an electron in a hydrogen atom. Following the standard curriculum, they will even do complex mathematical calculations using quantum mechanics to make predictions. However, being able to use the concept is not the same as having a full understanding of the theory. Hardly anyone has understood the theory to the fullest and some phenomena are still part of ongoing quantum mechanics research. While quantum mechanics describes quantum particles' behavior with great precision, it remains unclear what that means for our view of electrons and chemical bonds themselves. For example: What is the real nature of electrons? What is the state of an electron in the bound state of an atom or a chemical bond? Does this state differ when we try to measure it or was it the same before the measurement?

What does that mean from a didactic standpoint? How can we expect students to understand why two atoms form a chemical bond, whereas chemistry experts take years to fully understand the nature of a chemical bond? Should we forget about the idea to learn about chemical bonds at all? Should we rather teach students simple heuristics to the end so that students "get to the correct result"?

I am convinced the answer to that question is no. While we must acknowledge the fundamental difficulties, we have to find level-appropriate concepts that provide students with rational explanations for microscopic phenomena. It is my strong belief that chemistry novices can be taught level-appropriate concepts that explain the fundamental behavior of the smallest particles.

Summary

To sum up: There are three main types of strong bonding situations and weaker intermolecular forces. Since we can never actually see the small particles that make up matter (i.e. atoms, ions, or small molecules), the concepts to explain how those particles hold together are prone to misconceptions and overgeneralizations. While surface characteristics of some substances might be very similar, the bonding situation does not necessarily have to. To rationalize everyday phenomena, like melting and boiling temperature of substances, or to make predictions of substance properties students need to obtain a solid understanding of the three different bonding concepts as well as the intermolecular forces and methods of how to decide which bonding type might be present in a substance of interest. Additionally, the language used to describe the particle world of matter makes use of terms known from daily life and is not consistent throughout all chemistry textbooks. Arguably the most challenging part about the instruction of chemical bonds is finding level-appropriate models for chemistry novices.

1.1 Need for Chemistry Education Research on Chemical Bonding

Understanding the attractive forces between the smallest particles and the chemical bonds formed between those is challenging for students. Chemistry educators face a complicated task in how to foster their students' understanding of this complex topic. Evidence-based suggestions from the chemistry education research community would provide relief for teachers to guide them when teaching about the chemical bond. To provide such guidance, four things are needed: (1) The identification of the major challenges for students when learning about chemical bonding, (2) appropriate assessment tools to quantify which difficulties and misconceptions persist after instruction on the topic, (3) methods and ready-to-use teaching materials that foster students' understanding of chemical bonds, and (4) empirical studies that evaluate the effectiveness of the proposed methods in a classroom setting in comparison to conventional instruction.

In past decades education research in mathematics and other sciences, like physics, have gotten more attention, while studies in the field of chemistry education are rarer: Many aspects of learning have not yet been investigated in the context of chemistry. However, some dedicated researchers have made important contributions to the aforementioned four points. The identification of difficulties for students when learning about chemical bonds (1) and persisting misconceptions (2) have gotten some attention in the late 1980ies: Interviewing students led to the development of two-tier multiple-choice questions on molecules and intermolecular forces (Treagust, 1988, 1995). This then paved the way for further interview studies to investigate students' understanding of chemical bonding and their mental representations (e.g. Boo, 1998; Coll & Taylor, 2001; Coll & Treagust, 2003; Taber, 1997). In their review article Ünal et al. (2006) summarize chemical education research studies conducted on the topic of chemical bonds: The majority of studies apply interviews as a qualitative measure (9 out of 15) and the others the aforementioned questionnaire. The studies confirmed what many chemistry educators suspected: Misconceptions were detected even after students were instructed on the topic of chemical bonds.

More advanced assessment tools, i.e. concept inventories, have been developed since for other topics in chemistry (see chapter 2 for a more detailed discussion on the diagnosis of students' understanding of chemical bonding and existing concept inventories for chemistry topics). However, what is still missing is an inventory that covers the conceptual understanding of all three bonding types: Hence there is a clear need for the development and evaluation of such an advanced assessment tool for the conceptual understanding of the fundamental topic of chemical bonding (point 2 from above).

Whereas research dedicated to the identification of challenges and misconceptions has progressed, more research is needed when it comes to methods of how to overcome those challenges. A suggestion given by Boo (1998) may still hold meaning today: ‘There is a need for further research leading ultimately to the revision of curricular materials and teaching strategies to enhance future chemists’ and scientists’ understandings of their subject’ (p. 578). According to a recent meta-analysis (Hunter et al., 2022), the majority of the research on teaching and learning of chemical bonding has since then consisted of studies applying qualitative measures (42 out of 48) with only three studies applying a pre- and post-test design with a control group. Eighteen studies made use of quantitative measures. Of those only seven studies went beyond the detection of misconceptions and are dedicated to (3) finding suited methods and developing a teaching intervention (or teaching materials) that improve students’ conceptual understanding of chemical bonding.

Cooperative learning (i.e. group work and jigsaw method) has been described as effective to improve understanding of chemical bonding in two classroom post-test intervention studies with limited group sizes (two classes with no pre-test): Acar and Tarhan (2008) found that cooperative learning in small groups led to higher results on a post-test than conventional teaching about metallic bonds. In comparison to conventional instruction, higher achievement scores were measured at the post-test for students learning with the jigsaw method: Students were assigned one bonding type or intermolecular interaction to prepare at home and presented and discussed their topic in groups in class (Doymus, 2008).

Additionally, a few studies focused on *computer-based activities* (i.e. interactive simulations or animations) to foster students’ understanding of chemical bonding (Frailich et al., 2009; Özmen, 2008; Özmen et al., 2009; Shahani & Jenkinson, 2016; Zohar & Levy, 2019). Their findings are in line with activity-based learning interventions having positive effects on learning outcomes (Freeman et al., 2014).

However, none of the aforementioned studies covers the topic of chemical bonding *comprehensively*: They rather only cover parts of chemical bonding theory or are designed as short interventions to enrich conventional teaching. Nahum et al. (2007) describe a more holistic approach by which chemical bonding and intermolecular interactions are framed as a continuum with increasing strength of attraction: They propose to incorporate a new curriculum based on the idea that all those attractions are understood as bonds, increasing in strengths (from van der Waals forces to hydrogen bonds to covalent bonds to polar covalent bonds and ionic bonds). Subsequent case studies building on that idea found that interviewed students were able to take up such a view on chemical bonding in close proximity to instruction, but fell back to alternate views of the chemical bond in upper classes (Joki & Aksela, 2018; Joki et al., 2015).

In summary, holistic approaches to reform or modify the curriculum on chemical bonding have so far either not been developed or have not been successful in sustainably increasing students’ conceptual understanding. Thus, it follows that there is a dire need for methods and ready-to-use teaching materials that foster students’ conceptual understanding of all types of chemical bonding. To provide evidence-based suggestions for chemistry educators, the effectiveness of such methods and teaching materials needs to be evaluated in classroom intervention studies and compared to conventional instruction.

1.2 Aims and Outlook to the Empirical Studies

Given the described challenges and lack of research, the overarching aims for my dissertation were to (1) *diagnose* and (2) *promote* students' understanding of chemical bonding. The aims, structure, and empirical studies of this dissertation are depicted in Figure 4. A brief overview is given in the following.

Figure 4: Overview of this dissertation's aims and empirical studies in upper secondary school (green) and at university (blue).

1. Diagnosing the Understanding (chapter 2)

In chapter 2, pre-existing concept inventories in chemistry are reviewed, then the development of the new inventory is described. The *Chemical Bonding Inventory* (CBI) was developed and optimized in the *piloting phase*, first at the upper secondary school (with the *Gymnasium piloting sample*) and then at the university (with the *university piloting sample*).

In the *evaluation phase*, the inventory was administered to first-year science university students: During two consecutive years, the conceptual understanding and persisting misconceptions were identified with the *university evaluation studies 1* and *2:* Results from these investigations led to the identification of students' major challenges when learning about chemical bonding and common misconceptions.

2. Promoting the Understanding (chapters 3 – 6)

In chapter 3, I discuss the potential of the *method of comparing and contrasting* to promote students' understanding of chemical bonding in light of related research stemming from category learning and mathematics education.

In chapter 4, first, the *development of the teaching materials* based on comparing and contrasting is laid out, before describing the *main ideas of the teaching unit* in more detail.

In the *Gymnasium intervention study* (chapter 5) the comparing and contrasting teaching materials were evaluated for their effectiveness in promoting conceptual understanding of chemical bonding and reducing misconceptions in upper secondary school compared to conventional instruction.

In the *university intervention study* (chapter 6) the comparing and contrasting teaching materials were condensed for a seven-lesson preparatory course for newly enrolled university science students. The materials' effectiveness in promoting conceptual change was evaluated with this intervention study.

2 Diagnosing the Understanding of Chemical Bonding

Where do the major difficulties and pitfalls lie when it comes to learning about chemical bonding? What are common misconceptions after students have been instructed on the topic in upper secondary school? In this chapter, I present a novel assessment tool to answer these questions.

For this matter, I first review pre-existing concept inventories in chemistry and elaborate why the development of a novel inventory for the assessment of conceptual understanding of all types of chemical bonds was necessary. In the following, the process of the development and optimization of the new inventory during the *piloting phase* is laid out. Next, the *evaluation phase* is described in more detail: The optimized version of the inventory was administered to science students newly enrolled at the university in two consecutive years (*university evaluation studies 1 and 2*). These studies intended to bring to light the *major challenges* students face when learning about chemical bonding and *identify common misconceptions*. In section 2.4, I describe the development of an adapted assessment tool for the investigation of students' *prior knowledge*. I conclude the chapter with a brief overview of the different assessment tools and inventories administered during the empirical studies of this dissertation project.

2.1 Introduction

The task of diagnosing the students' understanding of scientific concepts has challenged researchers in the past decades. In the 1980s, education researchers began to design multiple-choice items based on results from interview studies with students of the target group to address the challenge. The aim of such *diagnostic assessments* (i.e. a multitude of such items) was to elicit whether students developed scientifically appropriate models of a certain topic. Treagust (1988, 1995) was one of the first to apply such a strategy to evaluate for possible misconceptions in the field of chemistry education. Thereby two-tier multiple-choice items (i.e., yes or no questions with several justification options) were used. Such *diagnostic assessments* can be seen as the precursors to the well-known class of *concept inventories*. After Hestenes et al. (1992) published the *Force Concept Inventory* (FCI) many disciplines started to design and publish such inventories in their respective fields. The *Chemistry Concept Inventory* (CCI) was the first in the field of chemistry education designed by Mulford and Robinson (2002). At present, a multitude of inventories has been published for various chemical concepts (Brandriet & Bretz, 2014; Bretz & Linenberger, 2012; Bretz & McClary, 2015; Dick-Perez et al., 2016; Luxford & Bretz, 2014; Wren & Barbera, 2013, 2014).

Scope of Existing Inventories on Chemical Bonding

To diagnose the students' understanding of chemical bonding, I was looking for an appropriate inventory. Inventories using a multiple-choice format that cover chemical bonding (Luxford & Bretz, 2014; Nimmermark et al., 2016; Othman et al., 2008; Tan & Treagust, 1999) or general concept understanding in the field of chemistry (Mulford & Robinson, 2002) were requested from the authors or retrieved from journals. In the following, they were assessed for their suitability for the intended studies (see Table 1). A closer look showed that three out of five assessment instruments focus strongly on the theme of particle nature of matter, i.e. the understanding of the behavior of the smallest particles and how chemical compounds are built up, or structure-properties relations. None of the inventories cover all three types of bonding. Especially the understanding of metallic bonding is not subject to evaluation by any of the inventories. The *Bonding Representation Instrument* (BRI) by Luxford and Bretz (2014) seems to cover at least covalent and ionic bonding in sufficient depths with five and eight items, but as the name of the inventory is indicating, the level of investigation is the understanding of the *representation* rather than the understanding of the underlying concept of bonding. The students are asked in nine out of thirteen items to elaborate on a certain representation (e.g. what kind of bonding is present in a certain illustrated model) or give insights into what a certain representation might indicate (e.g. a line between two atom symbols). Since this project aims to evaluate the students' conceptual understanding of chemical bonds after their instruction at the gymnasium level, the BRI is not suited for the intended task. To the best of my knowledge, an inventory that evaluates understanding of all three bonding types for that category of students does not yet exist but needs to be designed and evaluated first.

*Table 1: O*verview of Chemical Inventories Including the Topic of Chemical Bonding.

Multiple-choice instruments covering chemical bonding	**covalent bonding**	**ionic bonding**	**metallic bonding**	**inter-molecular forces**	**particle nature of matter**	**structure properties relations**	**different topic**
Alternative conceptions of chemical bonding Tan & Treagust (1999)		**x (3)**		**x (1)**	**x (1)**	**x (3)**	
Chemical Concept Inventory (CCI) Mulford & Robinson (2002)				**x (1)**	**x (9)**		**x (8)**
Particle Theory Bonding Instrument Othman et. al (2008)		**x (1)**		**x (2)**	**x (5)**	**x (3)**	**x (1)**
Bonding Representation Inventory Luxford & Bretz (2014)	**x (5)**	**x (8)**					
Survey Instrument Nimmermark et. al (2016)	**x (1)**	**x (1)**		**x (1)**		**x (1)**	**x (1)**

Note. The Numbers in Brackets Indicate the number of items for a topic included in the inventory.

Development of the Chemical Bonding Inventory

How can the different types of bonds be described? Depending on the level of expertise, this will vary. Utilizing this idea, I developed a *multi-level scheme of conceptual understanding* for each bonding type. The following question guided the development of such an inventory: What is needed to be able to explain the different attracting forces to build up molecular, metallic, or ionic substances? I defined *key aspects*, i.e. sub concepts or need-to-know facts, to be able to understand the cohesion forces of the different bonding types. Since such an explanation can be given on different levels (e.g. superficial explanation, or with varying degrees of complexity). I structured the *key aspects* for the conceptual understanding of the bonding types into multiple levels. As an example, the conceptual understanding structure of the ionic bonding situation is given in Figure 5.

Ionic Bonding – Conceptual Understanding of Ions and Ionic Compounds

Level 1: key aspects
- Definition of an ion
- Salts are constituted of ions
- Salts are made up of metallic and non-metallic elements (formal)
- Identification of salts from the chemical formula of substances
- Detection of anion and cation from the chemical formula

Level 2: key aspects
- Information content of chemical formula of salts (empirical formula vs. molecular formula)
- Ionic compounds are not constituted of pairs of ions
- Detection of the correct visual model for the bonding situation of ionic compounds

Level 3: key aspects
- Understanding of the term *ionic lattice* and the reason behind cohesion of ions
- Number of bonding partners in ionic compounds (no directionality of bond)
- While boiling, ionic bonds are broken (no intermolecular forces as commonly observed in molecular substances)

Figure 5: Key aspects for the understanding of ions and ionic compounds organized in three levels with increasing complexity.

Based on this model, I thought of possible ways of how to assess those key aspects with items of differing formats. The key aspects of each item are given in the method section, p. 26 onwards.

Another source for items, questions, or distractors in multiple-choice items were naïve concepts or misconceptions: I thought of ways of how students might misrepresent some concepts or ideas and incorporate naïve concepts into their explanations of the chemical bond. Besides my own experiences in the classroom, I could rely on findings described in interview studies (e.g. Coll & Treagust, 2003;

Levy Nahum et al., 2010; Taber, 1998, 2003). The discussions with Dr. Juraj Lipscher (chemistry teacher for 32 years) gave rise to further ideas.

Scope of the Developed Inventory

The application of the inventory aims to evaluate students' understanding of fundamental concepts concerning chemical bonding. Thereby the concepts of the three bonding types, as well as intermolecular forces, and their relations, are investigated. The level was set in accordance with students' expected level of understanding after instruction at a Swiss Gymnasium, the highest track of the Swiss educational system. Because the investigated concepts are very fundamental to chemistry itself, it can be assumed that the topics investigated are similar on an international level as well. The inventory assesses the understanding of basic understanding and could be described as the minimum students should be able to have understood after having covered the topics of chemical bonding at secondary level 2. This means that the designed items only investigate the understanding of fundamental concepts concerning chemical bonds. Detailed knowledge about specific substances is not necessary to complete the inventory.

The inventory investigates the following:

- Sound description of the forces behind the attraction in different bonding situations
- Correct conceptual representation of the three bonding situations
- Ability to deduce the bonding situation present in a substance with only the chemical formula at hand
- Ability to deduce the correct intermolecular forces present in a substance
- Ability to distinguish intermolecular forces from chemical bonds
- Misconceptions concerning the chemical language used for teaching about chemical bonds

2.2 Method

Sample

The inventory was developed and optimized based on a *piloting phase* and then used in the main *evaluation phase* to elicit students' conceptual understanding with a total of four samples:

Gymnasium piloting sample consisted of a student cohort of 10th and 11th graders (*N* = 182, 102 female, 80 male, mean age of 17) from three different Swiss Gymnasiums, the highest track in the Swiss educational system. A total of 12 classes were recruited via teachers interested in my dissertation project and the possible findings. Students were not compensated for their efforts.

The ***university piloting sample*** consisted of 175 first-year university students (69 female, 106 male, mean age of 19.4 years old) attending their first tutoring lesson in the fall semester of 2019. The targeted group was highly selective: students with the study subject chemistry, chemical engineering, biochemistry, or interdisciplinary natural sciences (focusing on biology and chemistry or physics and physical chemistry).

The ***university evaluation sample 1*** consisted of 1017 science students (560 female, 457 male, mean age of 18.8 years) attending their first tutoring lesson in the fall semester of 2020. Students taking part in my study were enrolled in various science bachelor subjects at ETH Zurich (see Table 2 for an overview).

The ***university evaluation sample 2*** consisted of first-year university science students (*N* = 970, 595 female, 368 male, mean age of 19.9) at the beginning of their studies in the fall semester of 2021.

Table 2: Number of participating science students with their field of study

Field of study	*Evaluation Study 1 (2020)* *N*	*Evaluation Study 2 (2021)* *N*
Agricultural Sciences	53	33
Biochemistry*	21	58
Biology	77	93
Chemical Engineering*	24	31
Chemistry*	74	62
Earth and Climate Sciences	42	44
Environmental Engineering	73	57
Environmental Sciences	143	134
Food Sciences	63	69
Health Sciences and Technology	267	233
Interdisciplinary Sciences*	74	52
Pharmaceutical Sciences	106	104
	1017	**970**

Note: * Field of studies that were also assessed in the *university piloting phase* (2019),

Procedure

The research group of Elsbeth Stern and co-workers, as well as Andreas Vaterlaus, have already been successful in developing inventories in physics (Hofer et al., 2017; Lichtenberger et al., 2017) and biology contexts (Champagne Queloz et al., 2016). The author could therefore rely on colleagues' experience in the development of inventories.

A new inventory was developed and optimized in the *piloting phase* with the *Gymnasium piloting sample* and the *university piloting sample*. In the following, the inventory was administered to a large cohort (*university evaluation samples 1 and 2*) in the first week of university in two consecutive years (fall semester 2020 and 2021). The procedure is depicted in Figure 6.

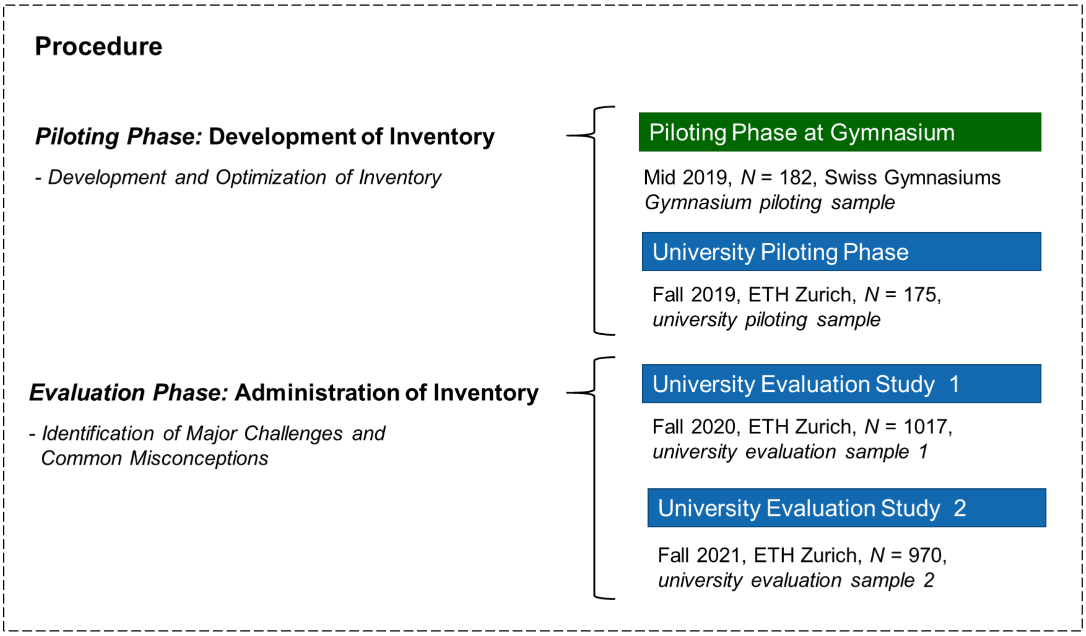


Figure 6: Procedure of the development of the inventory on chemical bonding with the piloting phase (Gymnasium and university, 2019) and the main assessment phase (university evaluation studies 1 and 2)

Piloting Phase

The ***piloting phase at the Gymnasium*** consisted of three rounds of investigations between April and July 2019. I optimized the first version of the pen-and-paper inventory with students that had already been instructed on the topic of chemical bonds in three rounds. Items were evaluated for their effectiveness and open-answer questions were used to gather more information about potential persisting misconceptions. After each round of inventory application, the students' feedback was implemented.

The ***university piloting phase*** (fall semester 2019) was used to assess whether a selective group of first-year university students studying chemistry-related subjects before attending lectures had deficits in the understanding of chemical bonding. Thereby the inventory was further optimized and enriched. Additional answers to open-format questions were gathered and evaluated for potential usages as distractors. The idea was to elicit whether this highly selective group of students enrolling at this prestigious science university and choosing the field of chemistry (or closely related) also held misconceptions and if so, to what extent. Additionally, it was an opportunity to evaluate whether the questionnaire with fewer open questions was applicable to a larger cohort. The participants were asked to fill out the pen-and-paper questionnaire during their first practice lesson with teaching assistants. The students were distributed into rooms with approximately ten to twenty students and supervised by a tutor. Since the evaluation took place in person and was an official part of the tutoring lessons the participation rate was exceptionally high (i.e. approximately 90 % of all students enrolled). During the assessment, the teaching assistants projected a periodic table on the screen (see appendix 1.1). No other means of support were allowed. Students were informed that the investigation was conducted to realistically assess their understanding and that the evaluation was anonymous without any negative consequences for their studies. To foster their motivation to participate with their best effort they were promised personalized feedback via an anonymous code they generated themselves.

Evaluation Phase

In ***university evaluation study 1*** (fall semester 2020) the inventory was administered to a larger cohort of university science students (*university evaluation sample 1*). The aim was to assess students' level of conceptual understanding and to identify common misconceptions held by a wide range of science students before attending lectures at university. The investigation was conducted in high accordance with the procedure of the *university piloting phase*. There was one major change: The inventory was no longer a pen-and-paper assessment at that point to cope with the large amount of data collected. The online-based questionnaire software of *Qualtrics International Inc.* was used to make the CBI accessible via a web browser. Even though the questionnaire was filled out online on every student's laptop, the evaluation was still conducted in person with a tutor supervising students. The students were asked to bring a laptop to the first exercise lesson to do the questionnaire. Tutors were circulating to prevent students from utilizing further support (e.g. other tabs in the internet browser). Students from five fields of study (Agricultural Sciences, Earth and Climate Sciences, Environmental Engineering, Environmental Sciences, and Food Sciences, 374 out of 1017 students) were given a shortened version of the inventory (i.e. four items less) due to time restraints in the first practice lessen.

University evaluation study 2 (fall semester 2021) was mainly a replication study. Three more items on intermolecular forces were implemented for this investigation. Due to the *university intervention study*, one week before the semester started, the 293 participants of the previously held preparatory course had to fill out the inventory before the start of the intervention. This was done online at home. The participating students' pre-test was hence used as their assessment at the semester start. For details on the *university intervention study* and data collection see chapter 6. Based on the findings of *university evaluation studies 1 and 2*, I attempted to make inferences on the major challenges students face when learning about chemical bonding.

Pilot Study

To the best of my knowledge, there had not been any published investigations into students' understanding of chemical bonding or misconceptions in Switzerland at the Gymnasium level or any other level. The first step was hence to identify whether there were any misconceptions present and to get feedback on students' conceptual understanding after having been instructed on the topic. Additionally, the inventory needed to be evaluated and optimized on different levels:

1. Wording of the questions: Students were prompted to give feedback when they did not understand the question.

2. Identify wrong answers and misconceptions: Open-format questions led to additional distractors.

3. Identify interesting wrong answers: Closed-format questions with many possible answers could be shortened when some answers were not attractive to students or too simple to identify as incorrect.

4. Conversion from open to closed-format question: To evaluate students' understanding in a short amount of time and on different levels more closed-format questions were needed. Therefore some open-format questions could be replaced by multiple-choice items step-by-step.

The first investigations and optimizations were conducted at the Gymnasium level (N = 182, *Gymnasium piloting sample*, see sample section for details). As aforementioned, the first version of the inventory was optimized in three rounds during the *piloting phase at the Gymnasium*. In the second step, the optimized inventory was administered during the piloting phase at the university (N = 175, *university piloting sample*, see sample section for details).

Piloting Phase at the Gymnasium

The preliminary inventory with many open questions was administered to the *Gymnasium piloting sample* revealing that misconceptions do persist after being instructed on the topic of chemical bonds. The open questions gave rise to many new distractors. Open questions were also used to validate pre-existing distractors known from interview studies and my own experiences as a chemistry teacher. Students' remarks about questions or answer options were taken into account when improving the inventory. The preliminary version of the inventory consisted of 29 items, eight open-format questions, and additional items with tasks to elaborate on why they chose an option to validate if the students came to the right solution because of the correct reasons. Two items were dropped due to many misunderstandings. Two open-format-questions were transformed into closed-format questions and distractors that were not chosen often were taken out of the inventory and sometimes replaced with student answers from open questions. Two students, having finished upper secondary school with no further chemistry training, and without any involvement in the study were asked to fill out the inventory and then elaborate on their decision-making. I interviewed the students one by one and asked them why they chose certain options and additionally asked, what they thought the different statements meant. The thinking-out-loud protocol helped to increase the validity of the inventory by reducing possible misunderstandings of item questions, statements, and distractors.

University Piloting Phase

The evaluation of the questionnaires revealed two things: The questionnaire was also applicable to a larger cohort and the transformation to the multiple-choice format was successful. Additionally, I found that even highly interested students (chemistry majors and closely related fields of studies) lack fundamental knowledge concerning the basic conceptual understanding of chemical bonds. Indications of common misconceptions concerning sodium chloride for example were found in this highly selective cohort. If asked how sodium and chloride are represented in a rock salt crystal (NaCl), 29 % would say that they are represented as a *sodium chloride molecule*. Arguably even more revealing was the fact that 16 % ticked the answer box “wrong” in front of the statement that sodium chloride is represented as sodium ions and chloride ions. Given the fact that sodium chloride is the most prominent of all ionic compounds. Even though we were expecting the prevalence of misconceptions also for this highly selective group the extent of students showing uncertainties for the fundamental concepts elicited the idea to enlarge the investigated cohort with students studying subjects with less chemistry in their future field of study (see *university evaluation studies 1 and 2*).

The collection of the larger amount of data allowed for a first psychometric analysis of the inventory. The analysis revealed items with potential weaknesses concerning wording or negative internal consistencies, which were then looked at in more detail. The pilot study’s insights were used to arrive at an inventory with 25 items, described in the following section.

New Inventory on Chemical Bonding

The pilot phase yielded an inventory for the assessment of students’ understanding of chemical bonding. In the following, I will refer to the inventory as the *Chemical Bonding Inventory* (CBI). A short overview of the most important features of the developed inventory is given first. Next, I present the two most important measures: the *total* and *subscore* as a measure for conceptual understanding, as well as the measurement of the *frequency of misconception* (FoM). Scoring and the different assessment item styles are presented last.

Measures of the CBI

The CBI assesses (A) students’ *conceptual understanding* of chemical bonds and their relations to intermolecular forces and (B) the prevalence of *misconceptions* on the topic of chemical bonding. Conceptual understanding is measured with the *total score* and *subscores.* The prevalence of misconceptions is measured using the *frequency of misconception* measure.

Total score and subscores are increased every time a student chooses all the correct options for the statements under a question. If a student chose all correct in item Q1 (see Figure 7), one point will be awarded for the ionic bonding subscore, since the item assesses key aspects of the ionic bonding. The total score is also increased by one. 25 items of different formats are used to deduce information about students' *conceptual understanding* of chemical bonds (A in Figure 7). The conceptual understanding is then represented with a *total score* (sum of all items) and *subscores* (sum of items assigned to the different subscores, e.g. ionic bonding). Detailed descriptions of the total score and subscores are given on the next page.

The frequency of misconception **(FoM)** is measured using the *distractors* of the items. A tendency for misconceptions is detected when students chose incorrect options, i.e. distractors. Every time such an incorrect option associated with a certain misconception is chosen, the count is increased by one (B in Figure 7). If a student chose the true option for the second statement (light blue cross in Figure 7), the count for the misconception *salt as a molecule* is increased by one for example. Single incorrect answers pointing towards the prevalence of a certain misconception were counted and added up for all items of the CBI resulting in a mean score for every misconception. Dividing by the total number of distractors taping into this misconception, a *frequency of misconception* (FoM) was calculated for different identified misconceptions. A more detailed description of this measure can be found on page 29 onward.

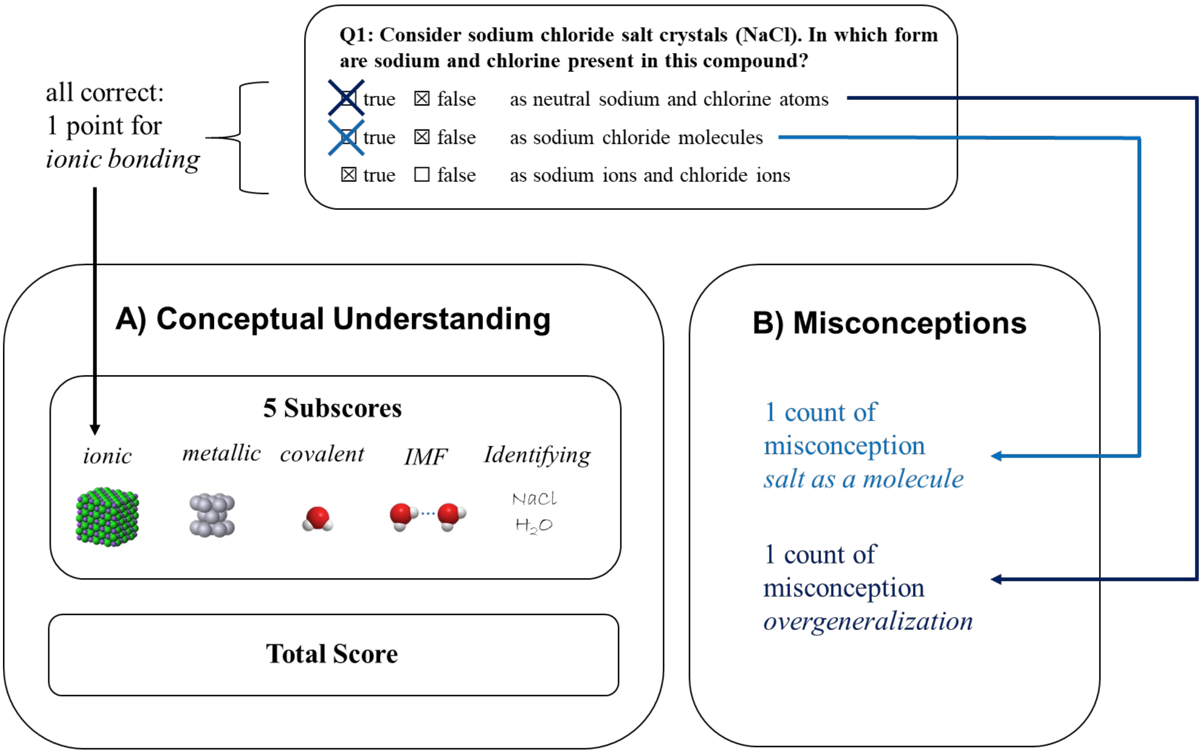


Figure 7: Assessment of conceptual understanding (A) and detection of misconceptions (B) in item Q1

Total Score and Subscores as a Measure for Conceptual Understanding

The conceptual understanding is assessed using the *total score* and *subscores*. Utilizing the fact that each item can be assigned to a certain bonding type or intermolecular force subscore, more detailed assessments can be made. The assignment of the items to the subscores is done according to Table 4, p. 37. A more detailed description of the points given and associated with subscores is shown in appendix 1.2. In the following, I outline what the different scores stand for and how they are built.

Total Score (31 points)

The total score, i.e. the sum of all 25 items, leads to a maximum score of 31 points. This score can be used to assess the conceptual understanding of *all bonding types*, the *intermolecular forces* as well as the *ability to distinguish between them*.

Ionic Bonding – Conceptual Understanding of Ions and Ionic Compounds (12 points)

Q1: Salts are constituted of ions
Q3: Information content of chemical formula of salts (empirical formula vs. molecular formula)
Q6: NaCl does not build NaCl molecules or subunits of ions (in detail)
Q7: Definition of an ion
Q8.1: Ionic compounds are not constituted of pairs of ions (shown for KCl)
Q8.2: Understanding of the term *ionic lattice* and the reason behind the cohesion of ions
Q11.2: Identification of salts from the chemical formula of substances
Q11.4: Detection of anion and cation from chemical formula
Q13: Number of bonding partners in ionic compounds (no directionality of bond)
Q19: Detection of the correct visual model for the bonding situation of NaCl
Q22: Salts are made up of metallic and non-metallic elements (formal)
Q25.2: While boiling, ionic bonds are broken (no intermolecular forces in salts)

Metallic Bonding – Conceptual Understanding of Metallic Substances (8 points)

Q5: Reasoning for cohesion forces in metals
Q11.1: Identification of metals from the chemical formula of substances
Q12: What kind of bonds are present in metals, i.e. no covalent bonding, no ionic bonding
Q14: Behavior of valence electrons in metals
Q15: Understanding of the term *metallic lattice*
Q20: Metals as a visual model
Q22: Metallic substances are exclusively made up of metallic elements (formal)
Q25.2: While boiling metallic bonds are broken (no intermolecular forces in metals)

Covalent Bonding – Conceptual Understanding of Molecular Substances (8 points)

Q3: Definition of the term *molecule*
Q9: Ability to identify the number of valence electrons of an element
Q10: Ability to deduce the number of covalent bonds a non-metallic atom can form
Q11.3: Identification of molecular substances from the chemical formula of substances
Q16: Covalent bonds hold atoms together in molecules (no other type of bond or IMF)
Q21: Reason for the cohesion of atoms of a water molecule (covalent bond vs. IMF)
Q22: Molecular substances are exclusively made up of non-metallic elements (formal)
Q25.1: While boiling, intermolecular forces are broken, covalent bonds are not

Intermolecular Forces (IMF) – Conceptual Understanding of Interactions between Molecules (8 points)

Q17: IMF are present in molecular substances only
Q18: Relative strength of IMF compared to chemical bonds (metallic, ionic, covalent)
Q23: Evaporated water in a visual model
Q24: Ability to order a series of substances according to their boiling point (molecular substances exhibiting intermolecular forces with lower boiling points compared to ionic and metallic substances)
Q25.1: IMF are counteracted in the gaseous state of molecular substances (covalent bonds still intact)
Q25.2: There aren't any IMF in metals and salts, hence while boiling the ionic and metallic bonds need to be broken apart.
Q25.3 Ability to identify the correct IMF present in a substance

Identification – Ability to Deduce the Substance Class from Chemical Formula (7 points)

Q11: Given a series of chemical formulas, the ability to assign the correct substance class
Q22: Formal understanding of metallic/non-metallic combination possibilities to form different types of substance classes, i.e. metals, salts, or molecular substances

Note: Items relevant to the Identification subscore are also used for other subscores

Assessing the Frequency of Misconception

I evaluated all individual incorrect answer options (distractors) for their possible association with a category or misconception. Single incorrect answers pointing towards the prevalence of a certain misconception were counted and added up for all items of the CBI resulting in a mean score for every misconception. Dividing by the total number of distractors taping into this misconception, a *frequency of misconception* (FoM) was calculated for different identified misconceptions (see Table 3).

Table 3: Total Number of Distractors Associated with a Misconception in the Chemical Bonding Inventory

Misconception	Total Number of *Distractors* in the *Chemical Bonding Inventory* (CBI)
Overgeneralization	21
NaCl molecule	11
Subunit or pairs in salts	6
IMF in metals	3
IMF in ionic compounds	2
IMF within molecules	4
Ionic lattice	1
Metallic lattice	4

This led to a powerful additional assessment measure beyond the *total score* for the assessment of conceptual understanding. What are the advantages of the FoM as an additional measure?

1. Measure between completely correct and wrong

Students can have different degrees of conceptual understanding and differ in their level of prevalence of different misconceptions. Since only all-correct items will lead to a point in the concept scores (see next section about scoring for more details) the inventory will not differentiate between partially correct and incorrect. The reality is that students on the level between being a layman and becoming more of an expert in the field (e.g. science students) will exactly be in that zone of transition. Neglecting the FoM measure would hence decrease the power of detection.

2. Increase in the validity

Instead of only measuring a certain misconception once it is measured multiple times within different items in different contexts. With this, the validity of findings by such a procedure is increased and a more realistic picture of the prevalence of a certain misconception can be obtained.

3. Comparability of misconceptions

Standardizing (dividing by the total number of distractors taping into a misconception) allows for a faster comparison and read-out of change effects between timepoints (e.g. post-test to follow-up). However, I caution the reader to not interpret too much into the comparison between different misconceptions. The inventory’s primary objection was to evaluate conceptual understanding. The implementation of misconceptions was an important part of it: Students gave incorrect answers full of misconceptions and such answers were added or kept in the inventory as distractors if the option was chosen by other students in the following. Some misconceptions are present in many distractors (sometimes more than one in one item) whereas other misconceptions were only assessed with a few appearances in distractors.

4. High utility as an assessment tool for research
The single misconceptions can also be assessed by looking at all the individual answers but the FoM measure allows for a faster review of those and gives a more balanced reading without giving one single distractor with a potential confounded error too much emphasis. I make extensive use of this tool in this work as is shown in the following chapters.

Scoring of Items

Each item evaluates one *key aspect* of the conceptual understanding of a bonding type. As previously stated, I used a multi-level-scheme of understanding with different ideas or concepts that are needed to elaborate competently about the different types of bonding or intermolecular forces. Students were instructed to assess each statement individually (multiple answers correct are possible). Therefore, I decided on rewarding 1 point only if all answer options were answered correctly.

Q1 (see Figure 8) for example evaluates if students have understood the general idea of ionic bonding:
Key aspect: Salts consist of charged atoms, i.e. ions.

The following sub aspects are needed to be rewarded 1 point:
1. NaCl is an *ionic compound* / *a salt* (strong hint with the name "salt", a well-known substance)
2. There are *ions* present in an ionic compound (option 3, true)
3. The atoms are *not neutral* (option 1, false) → follows from 2.
4. There aren't any NaCl molecules in a NaCl crystal (option 2, false) → no pairs or subgroups, no covalent bonds

Q1: Consider sodium chloride salt crystals (NaCl). In which form are sodium and chlorine present in this compound?

☐ true ☒ false as neutral sodium and chlorine atoms

☐ true ☒ false as sodium chloride molecules

☒ true ☐ false as sodium ions and chloride ions

Figure 8: Item Q1 of the inventory, assessing the aspect "salts consist of charged atoms, i.e. ions" for the conceptual understanding of ionic bonding

Note: In the first evaluations I was using a different scoring method: Every line (true/false) was rewarded a point. I finally decided against such a scoring because of three reasons:

1. Content related: multiple aspects needed for the understanding of key concepts
I argue that different sub-aspects need to be understood to have a decent conceptual understanding of a key concept. Often a concept is more complicated than just understanding *one* fact. Therefore a measure for conceptual understanding should take multiple statements into account. For example, I would argue that you are not considered to have understood the ionic bonding situation well if any of the three statements of Q1 are assessed incorrectly. To illustrate this: Students would even get two out of three points when they would state atoms are *neutral* and present as *ions at the same time* or decide all statements are wrong. I argue a more strict measure is needed when we want a valid measure of conceptual understanding.

2. One point for each key aspect
Some items have more answer options than others. Q1 would reward a maximum of three points with the alternative scoring method, while Q7 (Assessment of students' understanding of ions, as positively or negatively charged ions) would reward a maximum of five points. While both aspects are important to be understood to have a clear picture of the ionic bonding situation, it is also apparent that the key aspect evaluated in Q1 is at least as important as Q7's. The total scores value should hence also reflect that appropriately.

3. Guessing probability
Taking into account the *guessing probability* one can argue for the more strict scoring method. The chance of guessing everything right (and being awarded one point) in Q1 is 12.5 %, while students have a change of 50 % to earn one point with the point-per-line method.

Note: Although I am convinced that the chosen scoring leads to higher validity, it must be stated that the main findings were observed regardless of the scoring method, i.e. the same trends and identified challenges for students have been observed in the prior samples before applying the stricter scoring method.

Advantages of Using Different Question Formats

The number of maximum points per item, the format (i.e. multiple-choice or open-format), and style (e.g. True/False, Matrix, Ordering task), as well as the number of options students, had for each item are given in Table 4. There are arguments to be made for all items to be assessed in the same way (e.g. one question and four answer options with a True or False option). I actively decided against such an assessment during the process of evaluation in the *piloting phase at the Gymnasium*. The reasons are given in the following:

1. Some key aspects are better assessed with different formats

In theory, a homogenous assessment is desirable. But there is also a downside to it. A few aspects are really hard to assess with this simple method of questioning. If we want to assess students' ability to identify the type of substance from the chemical formula only (see Figure 9). There are only three classes of substance possible, when we include molecule-ions in the mix we get two additional terms to assess. It is inefficient to ask for each chemical formula on its own – only for the reason of the homogeneity of the questions. A matrix-table fits the task better.

2. Some key aspects have limited sub-aspects to evaluate

In the evaluation phase, I realized that there are simply only limited options for certain questions to find appropriate types of statements or answers to the questions. In some cases, it does not at all add to the question's validity to add more answer options. For example in Q1, there are only three valid options for sodium and chlorine to be represented in a salt crystal (see Figure 8): neutral atoms, molecules, or ions. With the option to cross multiple statements as correct, there is also the option to state that there are neutral atoms *and* ions at the same time. Other options were simply never mentioned by students and would therefore not add to the validity of the inventory.

3. Possibility to use illustrations of chemical bonding situations

There is only so much we can assess or describe in short statements as answer options. If we want to assess students' views of the bonding situation it is very valuable to directly do so by showing them different illustrations of the bonding situations (e.g. Q19, see Figure 10). All items with this assessment style are indicated as 'excluding/models' in Table 4, p. 37.

4. Limitation of evaluation time

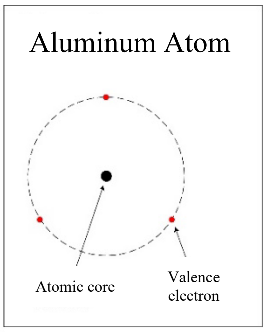
The core idea of inventories is to assess students' conceptual understanding *in a short period of time* with high precision. It follows from the above examples that different styles of assessment make use of the most efficient way of how to assess a key aspect in the least amount of time.

Q11: What is/are the right term(s) to use for the following substances?

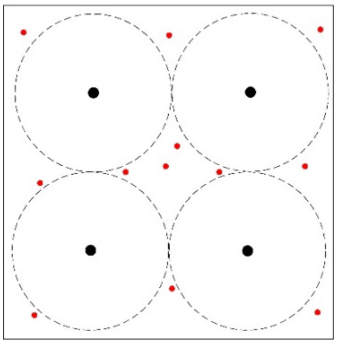
Chemical Formula	Metal	Ionic Compound	Molecule	Anion	Cation
PH_3					
$NaCl$					
NH_4^+					
LiF					
C_2H_6					
K					
$BeBr_2$					
CO_2					
HCO_3^-					

Figure 9: Q11 making use of the 'Matri' style of questioning

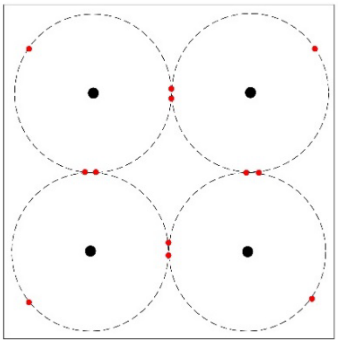
Q20: An isolated aluminum atom is shown below. Which of the pictures best reflects the state of the aluminum atoms when bonded, for example in an aluminum foil?



A.



B.



C.

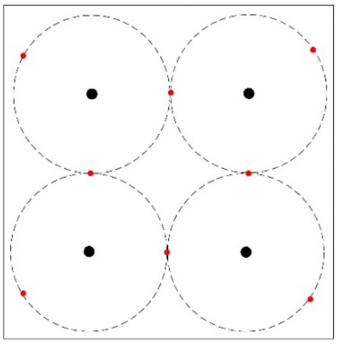


Figure 10: Q20 making use of the 'Exclusion / Models' style of questioning

Content Validity of the Chemical Bonding Inventory

The development of the inventory was supported and reviewed by a team of two Gymnasium chemistry teachers, two cognitive scientists, and a chemistry professor. As has been described in the development section of the inventory, the item construction was done based on fundamental concepts that are taught at upper secondary school and a multi-level scheme for the understanding of chemical bonds. Two chemistry teachers (with a master's in chemistry) not involved in this study were able to solve the inventory with a perfect score (except for item Q2, which has been excluded from the final version of the inventory).

Data Analysis

Data were analyzed with R (version 4.2.1, R Core Team, 2022) using the RStudio environment (version 2021.09.1, R Core Team, 2022). Packages used in the process were (in alphabetical order): afex (Singmann et al., 2022), data.table (Dowle & Srinivasan, 2021), effsize (Torchiano, 2020), EnvStats (Millard, 2013), eRm (Mair et al., 2021), lavaan (Rosseel, 2012), magrittr (Bache & Wickham, 2022), plyr (Wickham & Wickham, 2020), psych (Gick & Holyoak, 1983), PupillometryR (Forbes, 2020), readxl (Wickham & Bryan, 2022), semPlot (Epskamp, 2022), sjstats (Lüdecke, 2021), TAM (Robitzsch et al., 2022), tidyverse (Wickham et al., 2019).

2.3 Results and Discussion

During the *piloting* and *evaluation phase,* a total of 2344 students filled out a version of the inventory on chemical bonding. The detailed results of the *gymnasium piloting sample* ($N = 182$) and the *university piloting sample* ($N = 175$) are not given here because some items have been changed during the process of optimization and might be influenced by other items not being present in other versions of the inventory hence the comparability cannot be guaranteed. However, the data was valuable in guiding the development and optimization of the inventory and inspired the design of a multitude of additional items. Additionally, the data also elicited first insights into possible challenges students face when learning about chemical bonds.

Data collected during *university evaluation study 1* (fall semester 2020) stems from a shortened version of the CBI (CBI subtest). Hence total score, subscores, and FoMs differ or cannot be calculated as in *university evaluation study 2* due to some items missing. However, the datasets are highly comparable with very similar results for the common items of the two versions of the inventories. Since the student base was very similar (only differing in the year they started university) the data could be merged for the answering patterns of single items. When possible the datasets of *university evaluation studies 1* and *2* are merged (but always indicated in the following). In all other cases, the results from *university evaluation study 2* are presented (with the final version of CBI administered).

First, I present the results of the psychometric analysis of the items contained in the final version of the CBI. The test-retest reliability is given next, before presenting results from the conceptual understanding assessment (*total score* and *subscores* of *university evaluation sample 2*). In the following section profile analyses of the different subscores are discussed. The data collected during the *piloting phase* and *university evaluation studies 1 and 2* guided me in identifying five *major challenges* for students when learning about chemical bonding. In the last part of the results part, *common misconceptions* are presented and their frequencies (FoMs) are discussed.

Psychometric Item Analysis of the CBI

A complete version of the final inventory on chemical bonding (CBI) can be found in appendix 1.1. The inventory presented in this work consists of 25 items (see Table 4 for an overview). The psychometric analysis was conducted using *university evaluation sample 2* ($N = 970$, see p. 21 for more details on the sample). Item Q23 is taken out of the *Chemistry Concept Inventory* (CCI) developed by Mulford and Robinson (2002) and translated. The inventory's Cronbach's alpha was $\alpha = .84$. In addition, I calculated McDonald's omega based on polychoric correlations for the ordinal scale assuming one latent factor. This showed good internal reliability of the scale ($\omega_t = .92$). Item Q2 was excluded due to negative item discrimination ($r_{i(t-i)}$ of -0.02, in Table 4).

Table 4: Items of the Inventory on Chemical Bonding with their Associated Topic, Maximum Points, Mean (M), Standard Deviation (SD), Part-Whole Corrected Item-Total Correlation ($r_{i(t-i)}$), Assessment Style, and the Number of Options to Choose from. Assessed with University Evaluation Sample 2 (N = 970).

Item	Topic	Max Points	M	SD	$r_{\mathrm{i(t-i)}}$	MC	Style	Options
Q1	Ionic	1	0.56	0.50	0.50	yes	True/False	3x2
Q2*	Ionic	1	0.08	0.27	-0.02	yes	True/False	4x2
Q3	Covalent	1	0.06	0.24	0.13	yes	True/False	5x2
Q4	Ionic	1	0.30	0.46	0.27	yes	True/False	4x2
Q5	Metallic	1	0.06	0.24	0.30	yes	True/False	5x2
Q6	Ionic	1	0.17	0.37	0.53	yes	True/False	5x2
Q7	Ionic	1	0.89	0.32	0.20	yes	True/False	5x2
Q8.1	Ionic	1	0.66	0.48	0.29	yes	True/False	5x2
Q8.2	Ionic	1	0.06	0.24	0.26	yes	True/False	5x2
Q9	Covalent	1	0.77	0.42	0.19	no	Open Format Number	infinite
Q10	Covalent	1	0.66	0.48	0.29	no	Open Format Number	infinite
Q11.1	Metallic	1	0.70	0.46	0.36	yes	Matrix	9x1
Q11.2	Ionic	1	0.40	0.49	0.59	yes	Matrix	9x1
Q11.3	Covalent	1	0.42	0.49	0.57	yes	Matrix	9x1
Q11.4	Ionic	1	0.58	0.49	0.43	yes	Matrix	9x2
Q12	Metallic	1	0.21	0.41	0.48	yes	True/False	4x2
Q13	Ionic	1	0.07	0.26	0.17	yes	Excluding	5
Q14	Metallic	1	0.21	0.41	0.35	yes	True/False	5x2
Q15	Metallic	1	0.19	0.39	0.15	yes	True/False	5x2
Q16	Covalent	1	0.19	0.39	0.54	yes	True/False	6x2
Q17	IMF	1	0.19	0.39	0.17	yes	True/False	4x2
Q18	IMF	1	0.43	0.49	0.32	yes	Matrix	3x3
Q19	Ionic	1	0.60	0.49	0.47	yes	Excluding / Models	4
Q20	Metallic	1	0.58	0.49	0.48	yes	Excluding / Models	3
Q21	Covalent	1	0.21	0.40	0.55	yes	True/False	5x2
Q22	Identifying	1	0.41	0.49	0.41	yes	Matrix	3x3
Q23**	IMF	1	0.61	0.49	0.35	yes	Excluding / Models	5
Q24	IMF	2	0.45	0.65	0.29	no	Ordering Task	6 Substances
Q25.1	Covalent	1	0.25	0.43	0.20	yes	Matrix	4x3
Q25.2	Ionic/Metallic	1	0.26	0.44	0.48	yes	Matrix	2x6
Q25.3	IMF	1	0.01	0.11	0.15	yes	Matrix	3x6

Note. M = mean, SD = standard deviation, $r_{\mathrm{i(t-i)}}$ = part-whole corrected item-total correlation, IMF = intermolecular forces, * excluded, ** taken from CCI (Mulford & Robinson, 2002), *True/False* = multiple choice with possibly multiple correct answers (e.g. Figure 8, p. 31), *Open Format Number* = students are asked to provide a number, *Matrix* = rows and columns type of multiple-choice (e.g. Figure 9, p. 34), *Excluding* = multiple choice format with only one possible choice and one correct answer, *Excluding / Models* = models are depicted and students have to pick one (e.g. Figure 10, p. 34), *Ordering Task* = students are asked to order 6 substances according to their boiling point.

Test-Retest Reliability of the CBI

For interventions, the test-retest reliability is an important measure to reassure the effect on possible increases in conceptual understanding stems from the intervention and not the retaking of the test itself. The test-retest reliability was evaluated in the *university intervention study* (*N* = 293, see chapter 6 for more details). 293 students who took part in the *university intervention study* were a sub-sample of *university evaluation sample 2*. The CBI showed good test-rest reliability ($r(136) = .89$, $p < .001$) with two to five days between tests.

Assessing First-Year Science Students' Conceptual Understanding before Attending Lectures

The analysis of the total and subscores' solution rates elicited severe deficits in science students' fundamental understanding of chemical bonding (*university evaluation sample 2*). The overall solution rate was .36 (average total score of 11.10 of 31 points, SD = 5.40) for all investigated science students of *university evaluation sample 2* (see Table 5). Because the items assess absolute *basics* about chemical bonds this can be interpreted as a sign of a severe lack of conceptual understanding. The question was, whether the situation was different for very interested students with a chemistry background, i.e. students of chemistry, chemical engineering, biochemistry, and interdisciplinary sciences with a chemistry focus. For this sub-sample, the solution rate rose to .44 which is still not great considering the selective sample.

Table 5: University Students' Total Scores and Subscores for Conceptual Understanding

		University Evaluation Sample 2 *N* = 970			Chemistry and Biochemistry Students *N* = 203		
Score	Max Points	M	SD	Mean SR	M	SD	Mean SR
Total score	31	11.10	5.40	.36	13.70	5.52	.44
Ionic	12	4.57	2.01	.36	5.38	1.93	.45
Metallic	8	2.98	1.72	.37	3.44	1.7	.43
Covalent	8	3.05	1.74	.38	3.86	1.89	.48
IMF	8	2.19	1.56	.27	2.89	1.7	.36
Identification	7	4.29	1.99	.61	4.74	1.95	.68

Note. M = mean, SD = standard deviation, Mean SR = mean solution rate

Comparing the subscore's solution rates (SR in Table 5), it can be observed that the values were generally low for all subscores except the *Identification* subscore. How could that be interpreted? The *Identification* subscore is a measure of the ability to see a chemical formula and deduce the type of substance. This represents a mere superficial understanding of substances – but is still a necessary ability to acquire when learning about chemical bonds. It does, however, not change the general finding of a deficit in conceptual understanding in a large number of students starting their studies in a science major at university.

Confirmatory Factor Analysis of the Subscores

To further support the scale structure, a confirmatory factor analysis was run with four subscores (ionic bonding, metallic bonding, covalent bonding, and intermolecular forces). The identification subscore could not be modeled because it is also comprised of the other subscores. A Scree plot can be found in appendix 1.3. Confirmatory factor analysis with the *university evaluation sample 2*, yielded low model fit parameters (CFI = .862, TLI = .844, RMSEA = .043). The most commonly used interpretation of the CFI and TLI values indicates that values close to and above .95 are indicative of a good fit, higher than .9 indicating an acceptable fit, whereas RMSEA values below .06 are considered as parameters indicating a good fit (Hu & Bentler, 1999; West et al., 2012). These findings can be explained by the overall low solution rates for this sample: It can be safely assumed that the conceptual knowledge was not fully structured at that point. To validate this factor structure in a sample with higher conceptual understanding, I additionally used the post-test results of the administered CBI in the *university intervention study* (*N* = 293, a sub-sample of *university evaluation sample 2*, that was taught in a preparatory course, see chapter 6 for more details). After instruction on the topic, students' conceptual knowledge was more evolved and homogenous than at the pre-test. For this sub-sample, after instruction, the model showed a better fit to the data with parameters in the range of acceptable model fit (CFI = .90, TLI = .89, RMSEA = .032),

Profile Analysis of Subscores

A primary profile analysis of the subscores was conducted using *university evaluation sample 2*. The analysis did not yield profiles of particular interest: I found the first crossing of subclasses' subscore values with six and more subclasses (see appendix 1.4 for the depiction of the subclasses' profile analysis). Students that scored higher in one subscore typically also performed higher in other subscores. The profile analysis of the subscores with *university evaluation sample 2* hence points to the fact that the subscores are all measure concepts that are closely related. The finding also supports the formation of one *total score* for the topic of chemical bonding.

Identification of Major Challenges for Understanding Chemical Bonding

When we think of this evaluation as an assessment of the understanding of the absolute *basics* of chemistry, this evaluation brings to light a severe lack of understanding in all groups of science students, even in the most selective group of students. The question to answer is the following and represents one of the major findings of the diagnosing part of this dissertation project:

What makes it so hard to understand the basics of the concepts of chemical bonding?

1. The tendency to *overgeneralize* the covalent bonding type
2. The difficulty to *hold different bonding types* and their characteristics *apart*
3. The difficulty to hold *covalent bonds from intermolecular interactions* apart
4. A lack of understanding of the *cohesion forces* that hold together substances
5. The difficulty to use proper *chemical language*: chemical formula and use of specific terms

1. The Tendency to Overgeneralize the Covalent Bonding Type

The main finding of *university evaluation studies 1* and *2* is that students tend to overgeneralize. What does that mean? It is the tendency to take what you know from one concept and wrongfully apply or extend it to other concepts that do not support the same characteristics. In most cases, this is the *covalent bonding situation* that is very prominently represented in students' minds. They take what they know about the covalent bonding situation, i.e. neutral atoms covalently bound to form molecules, and wrongfully extend those characteristics to salts and metals. Many examples of overgeneralizations are given in the next section about common misconceptions (see p. 44 and onwards).

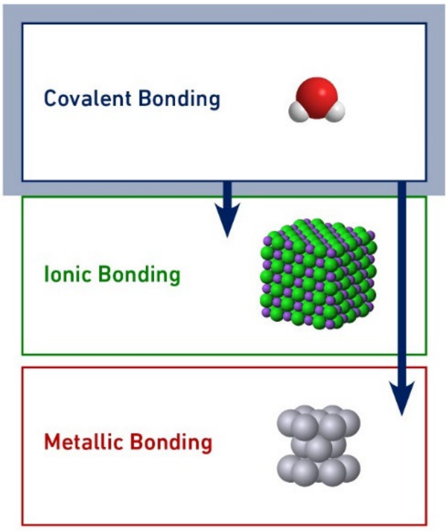


Figure 11: Illustration of the overgeneralization tendency observed in science students after instruction.

2. *The Difficulty to Keep the Bonding Types and Their Characteristics Apart*

The literature so far has pointed in the direction that students tend to overgeneralize the covalent bond (e.g. Hunter et al., 2022; Othman et al., 2008; Tan & Treagust, 1999). One could go so far as to state that some students do not realize at all that there is more than one bonding type, hence the confusion and misconceptions. This work's findings fully support previous findings, since the majority of misconceptions detected are following this pattern (see p. 44 and onwards for multiple examples). But it is also noteworthy that I discovered that students tend to confuse bonding situations in general: I calculated FoMs for the confusion of different bonding situations and/or their characteristics (e.g. students choosing a distractor that incorrectly describes an *ionic bonding* situation *as covalent*). Frequencies for the different confusion possibilities are depicted in Table 6.

Table 6: Frequencies of Misconceptions (Confusion of Bonding Situations), with the Mean (M) and Standard Deviation (SD) in University Evaluation Sample 2 (N = 970).

Bonding situation					
Correct	Described as	Max points	M	SD	FoM
Ionic	Covalent	6	1.20	1.28	0.20*
Ionic	Metallic	1	0.12	0.32	0.12
Metallic	Covalent	3	1.14	1.11	0.38
Metallic	Ionic	2	0.58	0.66	0.29
Covalent	Ionic	2	0.81	0.76	0.40
Covalent	Metallic	1	0.32	0.47	0.32
Covalent	IMF	6	3.02	2.02	0.50
		21	6.5	3.83	0.31

Note. M = mean, SD = standard Deviation, FoM = frequency of misconception, * lower value due to the exclusion of *salt a molecule* as a separate category of misconception (included 0.28)

The analysis clearly illustrates the general challenge for students to hold different bonding concepts and their properties apart: On Average, students agreed in 31 % of the cases with statements that stood for a description of an incorrect bonding situation or a characteristic typical for another bonding type, whenever it was presented to them.

3. *Distinguishing Between Intermolecular Forces and Chemical Bonds*

Taking a closer look at Table 6 (Covalent – IMF line) one finds that students also show difficulties when faced with the problem to distinguish between forces *within* a molecule (covalent bonds) and *between* different molecules (intermolecular forces). One explanation for this difficulty could be inherent to the process of evaluation of the strength of an intermolecular force: There are three types of intermolecular forces, and to assess which type is present students need to look *within* a molecule for polar bonds (i.e. high differences of electronegativity of two covalently bound atoms). Due to single polar covalent bonds within a molecule, the whole molecule has partial charges on two sides, potentially forming a dipole. Then they need to zoom out and look at the whole molecule; from that, they need to infer that molecules do attract each other, i.e. undergo an *intermolecular* interaction. Students do not seem to be made aware of this fact strongly enough when we look at the FoM of this misconception (see Table 7).

Table 7: Frequency of Misconception of Intermolecular Forces in Metals, Ionic Compounds, and within Molecules (N = 970, University Evaluation Sample 2)

Misconception	Max points	M	SD	FoM
IMF in metals	3	1.6	1.09	0.52
IMF in ionic compounds	2	0.9	0.82	0.45
IMF within molecules	4	1.5	1.05	0.38

Note. M = mean, SD = standard Deviation, FoM = frequency of misconception

Another interesting finding is that students tend to overgeneralize the existence of intermolecular forces within metals and salts (see Table 7). This can be explained with yet another overgeneralization: students overgeneralize the covalent bonding situation in general, assume molecules in all substances, and hence also incorrectly deduce that there must be intermolecular forces (see Figure 12). According to two review articles (Hunter et al., 2022; Ünal et al., 2006), the misconceptions that intermolecular forces occur in metals have not been described in the literature so far. Taber (1998) found in interview studies that students assume the existence of intermolecular forces in ionic compounds.

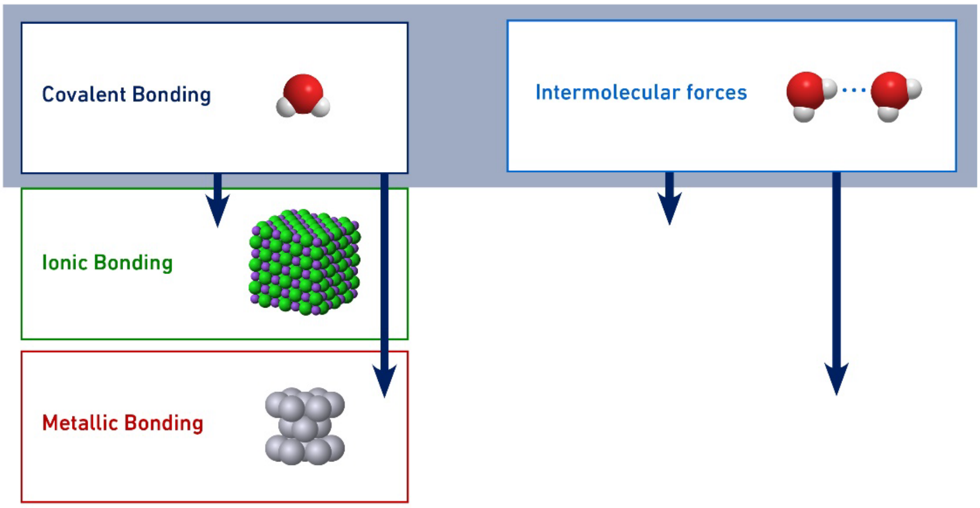


Figure 12: Illustration of the overgeneralization of the idea of the existence of intermolecular forces for ionic and metallic substances. Students assume molecules in the ionic and metallic bonding situation and wrongfully transfer their knowledge of intermolecular forces to metals and salts.

4. Lack of Understanding of the Cohesion Forces that Hold together Substances

Deduced from the results obtained by the *university evaluation studies 1 and 2*, I find evidence for students' lack of understanding of the cohesion forces at the fundamental level. What is it really that holds together the smallest entities in the three bonding situations? For many students this question seems to be more of a formality: Many students believe that for metals and ionic compounds this is the metallic respectively the ionic lattice (see p. 50 for an example). Others think that intermolecular forces hold together such substances (see paragraph above). Items investigating the fundamental reason why atoms and ions are held together are poorly solved throughout the whole inventory. Where does this stem from? Possibly, this has to do with the fact that level-appropriate models for understanding the reason behind the cohesion forces might simply not be provided. There is an inherent difficulty to consider: quantum mechanics is too complex for laypersons in chemistry. We, therefore, have to find level-appropriate models to help students grasp the fundamental reason why a substance holds together (see chapter 1 on the inherent difficulty of quantum mechanics and chapter 4.6 for a presentation of level-appropriate models used in the teaching unit developed in this project). Instead of having understood the fundamentals of chemical bonding, many students show signs of having incorporated formalism of why substances hold together: Some students seem to 'know' how to identify a bonding type by the chemical formula and 'know' that two dots (electrons) in the Lewis structure formula results in a covalent bond between atoms. When probed in more detail about the reason behind such heuristics, students often fail to give an appropriate answer. This hypothesis is supported by the finding that, for example, students in the *university evaluation sample 2* had a higher solution rate (.61) for the identification subscore whereas the other four subscores were lower (between .27 and .35, see Table 5, p. 38). Such superficial conceptual understanding is a gateway to further overgeneralizations and the prevalence of misconceptions.

5. The Difficulty to Use Proper Chemical Language: Chemical Formula and Use of Specific Terms

Students tend to overgeneralize also in the context of chemical language and the terms used to describe bonding situations: Molecules are not regarded as something unique to the covalent bonding situation but are rather seen as the prototype for all substances (see p. 49 for the unspecific use of the term and the concept of a molecule). The terms ionic and metallic lattice are given more than the actual meaning (the symmetrical spatial arrangement) and unwarranted explanatory power (see p. 50 for an example). Students also tend to deduce molecular formulas (and hence subunits) from chemical formulas of ionic compounds (see p. 47 for an example).

Identification of Common Misconceptions

In the following, prominent examples of misconceptions are presented to illustrate the challenges students face. The overarching major challenge is given in the title (brackets).

Salt as a Molecule (Overgeneralization)

The idea that sodium chloride, commonly known as (table) salt, forms molecules is widespread among students. Investigations into students' ideas about sodium chloride have replicated this finding multiple times (Coll & Taylor, 2001; Coll & Treagust, 2003; Luxford & Bretz, 2014; Othman et al., 2008; Özmen, 2004; Vrabec & Prokša, 2016). Depending on age, sample, and style of questioning the percentage of people stating that sodium chloride consist of molecules ranges from 18 % (grade 11/12, *N* = 330, Vrabec & Prokša, 2016) to 41 % (grade 9, *N* = 140, Othman et al. 2008). Those finding were the ones that initially caught my attention and led me to look closer into the topic of chemical bonding in the first place. But there are still many questions unanswered: What do students mean when they use the term *molecule*? Do they think of molecules as neutral atoms or ions paired in molecules? Are there maybe synthetic models that could be detected?

Q1 (see Figure 8, p. 31) assesses students' views of NaCl, using *university evaluation samples 1 and 2* (*N* = 1946), I found that NaCl is seen as *neutral* sodium and *neutral* chlorine atoms by 9 %, as sodium chloride *molecules* by 40 %, and 21 % disagree with the statement that NaCl is comprised of sodium *ions* and chloride *ions*. The more shocking result arguably was that approximately every fifth science student would say sodium chloride, i.e. *the* prototype of ionic compounds, is not comprised of ions. In a more selective sample, we still found these misconceptions in 29 % (NaCl molecules) and 16 % (no ions) of the investigated students (chemistry-related field of study, *university piloting sample*, *N* = 175, see p. 21 for details on the sample).

Identification of Synthetic Models of NaCl (Overgeneralization)

As previously stated, there are still open questions to be answered: How is the model of an ionic compound represented in students' minds? I designed items exactly to be able to elaborate more on this: Whereas item Q6 (see Figure 14) tests for synthetic models in the multiple-choice format, Q19 (see Figure 13) makes use of model visualizations of different NaCl models.

Q19: Four models of the NaCl salt crystal are shown below. Which one of them best represents the bonding situation in a salt crystal?

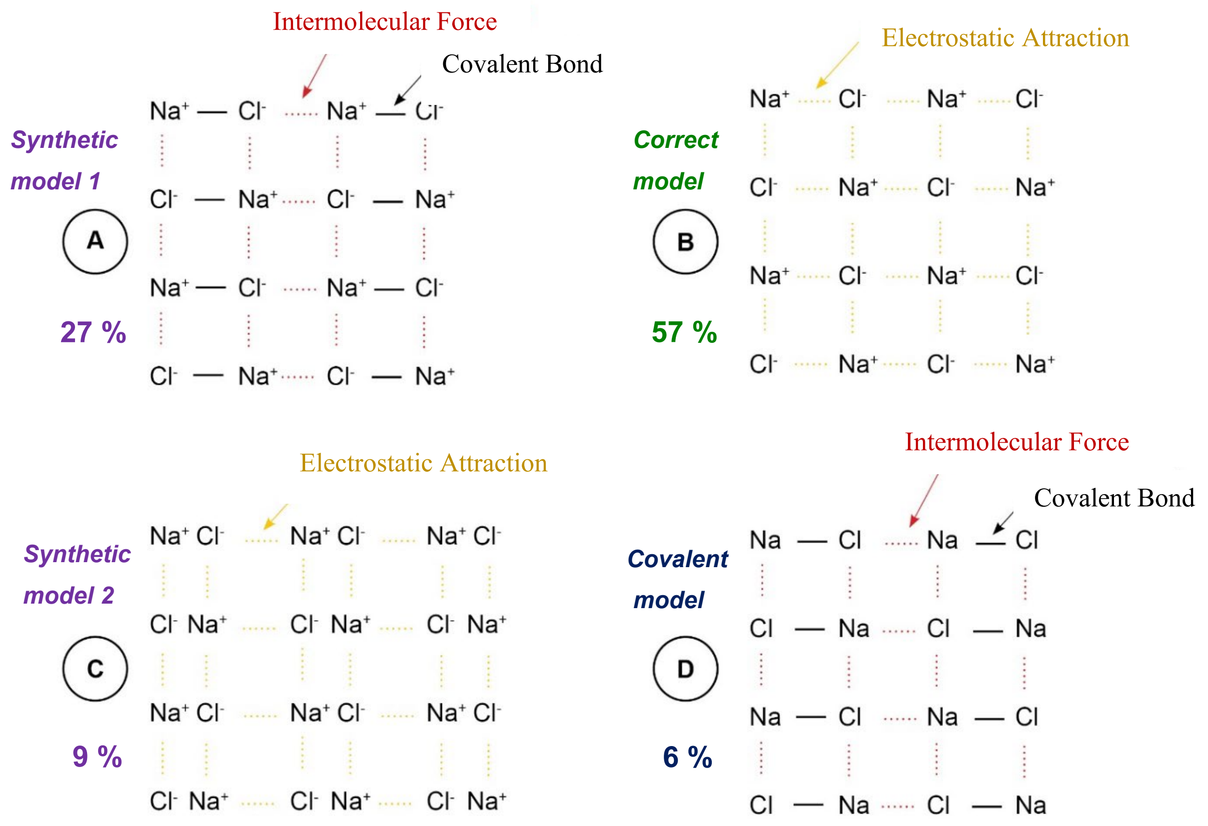


Figure 13: Q19 Testing for synthetic models in university evaluation samples 1 and 2 (N = 1946), Synthetic models A and C detected as well as the prevalence of misconception D (covalent model). Note: values rounded to integers

Q6: Sodium and chlorine react together to form sodium chloride (NaCl). Which of the following statements are true?

☐ true ☐ false 85 %	Sodium ions and chloride ions are formed, which attract each other due to their different charges.	
☐ true ☐ false 12 %	Neutral sodium atoms and neutral chlorine atoms cluster together in a lattice-like structure.	Covalent models
☐ true ☐ false 33 %	Sodium and chlorine atoms form electron pair bonds to form sodium chloride molecules.	
☐ true ☐ false 50 %	Sodium ions and chloride ions form, which combine to form sodium chloride molecules.	Synthetic models
☐ true ☐ false 58 %	One sodium ion and one chloride ion join together to form a unit.	

Figure 14: Q6 Testing for synthetic models in university evaluation samples 1 and 2 (N = 1946), Synthetic models A and C detected as well as the prevalence of misconception D (covalent model).

Investigating *university evaluation samples 1 and 2* (*N* = 1946), 57 % of the students chose the correct model, and synthetic models A and C were chosen by 27 % respectively 9 %. 6 % chose Option D, representing a complete covalent bond model of an ionic compound. Analysis of the solution rates of Q6 also revealed the prevalence of synthetic models. While 15 % disagreed with the fact that there are ions inside of a sodium chloride crystal, 85 % agreed. Agreeing to statements two and three points to the existence of covalent models for this ionic compound. A stunning 50 % agree with the idea of two ions combining to form a sodium chloride molecule. Additionally, 58 % agreed that there is some kind of unit formed out of one sodium and one chloride ion.

When I assessed chemistry students only (*N* = 62 out of *university evaluation sample 2,* see Table 8), I found that the students tended to shift more strongly towards the correct model (ionic bonding, 10 % more), and away from the covalent model 1 and 2 (being the most incorrect models). With the expected higher conceptual understanding of future chemists, one would exactly expect such a pattern.

Table 8: Distribution of Mental Model Representations of Sodium Chloride for all Science Students (N = 1946, University Evaluation Samples 1 and 2) and exclusively Chemistry Students (N = 62, Taken out of University Evaluation Sample 2)

Model	Description	Science Students (N = 1946, 2020 / 2021)	Chemistry Students (N = 62, 2021)
Correct model	ionic bonding	85 %	95 % (+10 %)
Covalent model 1	neutral atoms in a lattice	12 %	5 % (-7 %)
Covalent model 2	molecules	33 %	15 % (-18 %)
Synthetic model 1	ions form molecules	50 %	39 % (-11 %)
Synthetic model 2	ions form a unit	58 %	53 % (-5 %)

Note. Percentages in brackets indicate the difference in comparison to the science students.

The misconception that molecules are present in an ionic compound is assessed on 11 occasions when filling out the inventory (representing *covalent model 2* and *synthetic model 1*): in 33 % of the cases, the molecule distractor was chosen.

Note: I also evaluate the misconception with another ionic compound that is less known: potassium chloride (KCl). The results do not support the idea that students only assume molecules for sodium chloride (a well-known substance) but more probably incorrectly overgeneralize the molecule representation to all ionic compounds. A more evolved model (*synthetic model 2*) is also found in *university evaluation sample 2*: thinking that there must be some kind of *subunit* while knowing that this is not called a ‘molecule’, is another prominent misconception. The respective FoMs are depicted in Table 9 below.

Table 9: Frequency of Misconception for “Salt as a Molecule” and “Subunits or Pairs in Salts” (N = 970, University Evaluation Sample 2)

Misconception	Max points	M	SD	FoM
NaCl as a molecule	11	3.7	2.49	0.33
Subunits or pairs in salts	6	1.7	1.13	0.29

Note. M = mean, SD = standard Deviation, FoM = frequency of misconception

Chemical Formula of Ionic Compounds seen as Molecular Formulas (Overgeneralization)

Another example of the covalent bonding overgeneralization onto ionic compounds is observed when looking at Q4 (see appendix 1.1). Students wrongfully transfer what they know from molecules like water (H_2O) to ionic compounds like lithium bromide (LiBr). While it is completely correct that a water molecule is comprised of two hydrogen and one oxygen atom this is not true for salts. There is no subunit to be observed (as mentioned in the introduction). Even when we tell students that the substance at hand is an *ionic compound* we observe that 53 % (out of $N = 1946$) will wrongfully state that there are pairs in this compound, and 16 % say it is correct that there is some kind of *subunit*.

Overgeneralization in Metals

The overgeneralization of the covalent bond does not only occur in ionic but also the metallic bonding situation. When students ($N = 1946$) were asked what holds together a piece of copper, 34.6 % stated covalent bonds (German 'Elektronenpaarbindung'), 21.8 % anions and cations (i.e. ionic bonds), a stunning 62.7 % stated intermolecular forces (see next section) and 42.7 % said that it is not true that metallic bonds are different from ionic and metallic bonds (see Figure 15). The overgeneralization is starkly made visible with this item: Over 40 % of students stated it is wrong that metallic bonds differ from ionic and metallic bonds.

Q12: Copper is a metal. Which of the following statements are true about the bonds in a metal block of copper?			% incorrect answers
☐ true	☒ false	_Covalent bonds_* occur. (Elektronenpaarbindungen)	34.6
☐ true	☒ false	The atoms are present as positively and negatively charged ions.	21.8
☐ true	☒ false	The metallic atoms are held together by intermolecular forces.	62.7
☒ true	☐ false	The bonds in copper are different from ionic bonds as well as covalent bonds.	42.7

*Figure 15: Q12 with university evaluation samples' 1 and 2 (N = 1946) answers (only option 4 true), * the term 'covalent bonds' is not used in the German version. Instead, 'Elektronenpaarbindung' is used, a more specific term for bonds between two non-metallic atoms.*

Note: In German, there is the terminology 'Elektronenpaarbindung', i.e. a bond that is formed between two atoms with a pair of electrons being shared between two atoms. I used this terminology because it is more selective for molecules. On a more abstract level, metallic bonds can be described as similar to covalent bonds in terms of forming bonds over the whole metallic substance. Whereas one could correctly state that this is similar to a covalent bonding situation over the whole substance, it is not true that there are covalent bonds with electron pairs being located between two metallic atoms. This little episode illustrates the difficulty to translate inventories and stresses the importance of evaluation after being translated.

Intermolecular Forces in Metals and Salts (Overgeneralization)

When directly asked where intermolecular forces occur (see Q17 of the CBI, appendix 1.1) we find that approximately *one-third* of the students (*N* = 970, *university evaluation sample 2*) say *within metallic* and *ionic substances*. As previously discussed Q12 (see Figure 15, statement 3) is another example of overgeneralization (intermolecular forces also exist in metals). The more generalizable FoMs are depicted in Table 10. Of all distractors that can be chosen that tap into that misconception half are chosen. Methods of how to tackle these misconceptions are discussed in chapter 4.7.

Table 10: Frequency of Misconception of Intermolecular Forces in Metals and Ionic Compounds (N = 970, University Evaluation Sample 2)

Misconception	Max points	M	SD	FoM
IMF in metals	3	1.6	1.09	0.52
IMF in ionic compounds	2	0.9	0.82	0.45

Note. M = mean, SD = standard Deviation, FoM = frequency of misconception

Relative Strength of IMF in Comparison to Chemical Bonds

When students (from *university evaluation sample 2*) were probed on the relative strengths of intermolecular forces compared to chemical bonds uncertainties came to light: Students stated intermolecular forces were as strong, or stronger than chemical bonds (27.7 % for covalent bonds, 35.8 % for metallic bonds, 27.8 % for ionic bonds). Where did those uncertainties stem from? A possible explanation is that often direct comparisons of intermolecular forces with chemical bonds are not prompted. Typically, the topic of intermolecular forces is taught as a unit of its own. Thereby much emphasis is given to the differentiation and relative strengths of the three types of intermolecular interactions (van der Waals interaction, dipole-dipole interaction, or hydrogen bonding). Comparisons between intermolecular and covalent bonds are rarer, comparisons to ionic or metallic bonding are typically not prompted at all. Peterson and Treagust (1989) report that some students claimed intermolecular bonding was stronger than intramolecular (covalent) bonds, and Boo (1998) reported the finding of a student claiming that van der Waals forces were stronger than ionic bonding in semi-structured interviews. In chapter 4.7, I take up the described challenges and elaborate on how to possibly mitigate the formation of this alternative conception.

Usage of the Molecule Term (Terminology / Overgeneralization)

A challenge I have come across multiple times during my dissertation project was: What do students mean when they use the term ‘molecule’? What are defining characteristics of this term for students? To elicit how students define their molecule terminology I designed Item Q3 (see Figure 16).

Q3: On what does it depend whether an atomic ensemble is called a molecule?

It matters …		% incorrect answers
☒ true ☐ false	how many atoms are bonded together (at least two).	25.8
☒ true ☐ false	which types of bonds exist between the atoms.	39.0
☒ true ☐ false	whether atoms are in a charged or uncharged state.	72.7
☐ true ☒ false	that different kinds of elements are present.	20.6
☒ true ☐ false	which types of atoms (metallic/non-metallic) are present.	57.6

Figure 16: Q3 translated: Item to elicit more about students’ understanding of the term ‘molecule’. All statements are correct except statement 4. The percentages of incorrect answers are given for each statement for university evaluation samples 1 and 2 (N = 1946).

Whereas 25.8 % of students (*university evaluation samples 1 and 2*) neglected the fact that a molecule is defined as containing more than one atom, 39 % of the investigated students did not consider the bonding type between atoms when deciding whether an atomic ensemble is called a molecule or not. The charge of atoms or atomic ensembles is *the* defining characteristic to use the *ion* terminology instead of atom or molecule. However, whether atoms are charged did not seem to matter for an astonishing 72.7 % of students. The latter two findings are in line with some students applying the molecule term to ionic compounds like sodium chloride and a tendency to overgeneralize. 57.6 % of students did not seem to make the connection that the types of atoms (metallic/non-metallic) present in a substance do in fact matter, because it predicts the bonding type in a substance with great accuracy and hence determines whether the terminology *molecule* is appropriate or not. It must be noted that the ionic compounds containing charged molecular cations being exclusively made up of the non-metallic type (e.g. NH_4^+ with any anion) are not detected following the simple ‘*non-metal atoms only - resulting in molecules’* heuristics. In chapter 4.8, I present a possibility of how to sharpen students’ definition of the term *molecule*.

Ionic and Metallic Lattices are Given Incorrect Characteristics

(Terminology and understanding of cohesion forces)

The ionic or metallic lattice (‘Gitter’ in German) describes the symmetrical arrangement of ions or metallic atoms in a substance. Approximately half of the students in *university evaluation samples 1 and 2* (*N* = 1946) agree with statements that give the metallic lattice (‘Metallgitter’) meaning beyond the spatial arrangement. They agree with statements that see the reason for the cohesion forces of metallic atoms in the lattice itself (statement 1, in Figure 17), or even go so far as to say that the lattice is an *independent structure* to give the substance its stability (statement 3).

Q15: Consider a piece of copper. Copper atoms are arranged in a metal lattice. Which statements about the metal lattice are true?

			% incorrect answers
☐ true	☒ false	The metal lattice holds the atoms together.	52.3
☒ true	☐ false	The metal lattice describes the geometric arrangement of the atoms.	14.2
☐ true	☒ false	The metal lattice is an independent structure that gives copper stability.	50.1
☐ true	☒ false	The metal lattice holds the atoms in their positions.	50.0
☒ true	☐ false	The metal lattice results from the arrangement of the atoms.	86.5

Figure 17: Q15 translated: Items assessing students’ understanding of metallic lattices and the reason for the atoms to hold together in copper.

Students also show similar difficulties when it comes to the meaning of ionic lattices: 74.4 % of the students from the same sample agree with the statement that the ionic lattice is the reason for the ions to be kept on their positions (see Q8.2 of CBI, appendix 1.1). Taking into account all the distractors taping into lattice misconceptions the frequencies of misconceptions are depicted in Table 11.

Table 11: Frequency of Misconception for Lattice Misconceptions (University Evaluation Sample 2, N = 970)

Misconception	Max points	M	SD	FoM
Ionic lattice	1	0.8	0.423	0.77
Metallic lattice	4	2.3	1.25	0.58

Note. M = mean, SD = standard Deviation, FoM = frequency of misconception

Possible reasons for the strong prevalence of those misconceptions: (1) Students were not taught or did not fully incorporate a level-appropriate model for understanding the reason behind the cohesion forces of metallic atoms or ions, or (2) they transfer what they know from the term lattice

(‘Metallgitter’ in German) and physical models with metallic rods between the atoms (represented by balls). I am convinced that giving students a better understanding of why the ions or metallic atoms are held together (see chapter 4.6 for how to possibly tackle the misconceptions) and discussing the role and meaning of the term lattice in the context of chemical bonding is indicated. Exercises that target this prominent misconception are discussed in chapter 4.8.

2.4 Identification of Prior Knowledge of Chemical Bonding

What do students know about chemical bonding shortly before they are instructed on the topic? The *Gymnasium intervention study* made it necessary to develop an assessment tool before instruction (see chapter 5). Many items of the *Chemical Bonding Inventory* described in the previous section were simply not suitable for a cohort of students that have not been formally instructed on the topic. Students would have to guess the answer or would not even understand what was meant by the questions because they lack the necessary understanding of certain terms. I evaluated all the items of the *Chemical Bonding Inventory* for their possible use as a pre-test item in the *CBI pre-test*. Seven items were deemed appropriate for potential use as a pre-test item and could, later on, be used as link items for the pre-test, post-test, and follow-up test of the intervention (see Table 12, link items).

Additional items needed to be invented. The question to ask was: Which concepts build the basis for the understanding of the chemical bond? The answer is a sound understanding of the *structure of atoms* and *Coulomb’s law*. Students need to know about the elemental particles making up an atom (i.e. electrons, neutrons, and protons) as well as the attractive or repulsive interactions between them. The pre-test was evaluated with the *Gymnasium intervention sample* ($N = 308$ with completed pre-test, mean age of 17, see chapter 2.2 for details on the sample). An overview of all items is given in Table 12. The full pre-test can be found in the appendix 1.5. The inventory’s Cronbach’s alpha was determined at .69. In addition I calculated McDonald’s omega based on polychoric correlations for the ordinal scale assuming one latent factor. This showed good internal reliability of the scale ($\omega_t = .80$). An item unique to the pre-test is depicted below (no translation available).

Table 12: Items of the CBI Pre-Test Inventory with their Maximum Points, Mean (M), Standard Deviation (SD), and Part-Whole Corrected Item-Total Correlation ($r_{i(t-i)}$), Assessment Style, and the Number of Options to Choose from. Assessed with Gymnasium Intervention Sample (N = 308).

Item	Link Item	Max Points	M	SD	$r_{i(t-i)}$	MC	Style	Options	Topic
P1a		1	0.79	0.41	0.40	yes	True/False	4x2	Atomic Structure
P1b		1	0.61	0.49	0.33	yes	True/False	4x2	Atomic Structure
P2		3	1.96	1.18	0.38	yes	Matrix	3*5x2	Atomic Structure
P3		1	0.15	0.36	0.26	yes	True/False	4x2	Ionic
P4	Q7	1	0.63	0.48	0.27	yes	True/False	5x2	Ionic
P5*						no	Open format question		Ionic
P6	Q1	1	0.20	0.4	0.06	yes	True/False	3x2	Ionic
P7		1	0.34	0.48	0.28	yes	True/False	4x2	Ionic
P8	Q3	1	0.02	0.14	0.03	yes	True/False	5x2	Covalent
P9*						no	Open format question		Metallic
P10		3	1.20	0.92	0.41	no	Open format/numbers	infinite	Atomic Structure
P11	Q9	1	0.25	0.44	0.34	yes	Open format/numbers	infinite	Covalent
P12	Q4	1	0.19	0.39	0.04	yes	True/False	4x2	Ionic
P13a		1	0.34	0.47	0.53	yes	Excluding	5	Coulomb's Law
P13b		1	0.33	0.47	0.52	yes	Excluding	5	Coulomb's Law
P13c		1	0.76	0.43	0.19	yes	Excluding	5	Coulomb's Law
P14a		1	0.41	0.49	0.42	yes	Excluding	5	Coulomb's Law
P14b		1	0.81	0.39	0.20	yes	Excluding	5	Coulomb's Law
P15		1	0.31	0.46	0.35	yes	Open format/number	many	Coulomb's Law
P16	Q6	1	0.06	0.24	0.05	yes	True/False	5x2	Ionic
P17*						no	Open format question		Covalent
P18	Q20	1	0.46	0.5	-0.03	yes	Excluding / Models	3	Metallic
total		23	9.83	3.85					

Note. M = mean, SD = standard deviation, $r_{i(t-i)}$ = part-whole corrected item-total correlation, * not utilized in this assessment - intended for further research and validation purposes

P10: Im Chemieunterricht haben Sie bestimmt das Schalenmodell von Atomen kennengelernt. Geben Sie für die unten aufgeführten Elemente (S, K und Ti) für jede der angegebenen Schalen (K bis O) an, wie viele Elektronen sich darin befinden. Benutzen Sie dazu das zusätzlich ausgeteilte Periodensystem.

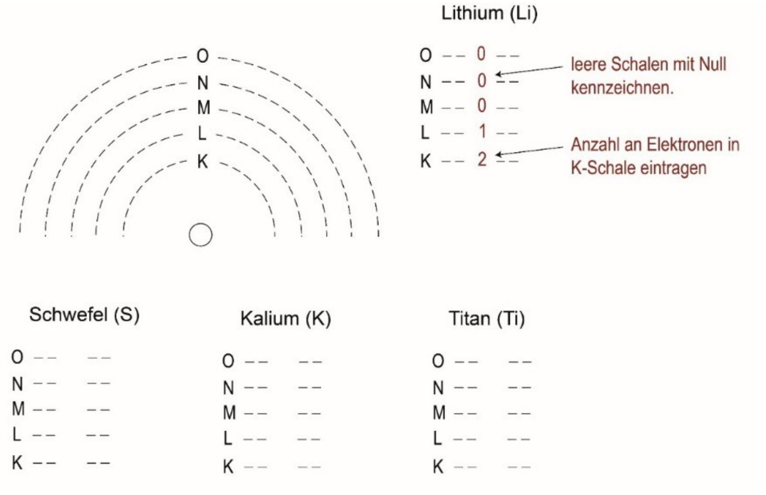


Figure 18: P10 – item from the pre-test for the evaluation of students' understanding of the shell model (atomic structure)

2.5 Summary of Tests Used in the Empirical Studies

In my dissertation project, I made use of different versions of the *Chemical Bonding Inventory* (CBI). This chapter aims to provide an overview for the reader. Table 13 depicts the total number of items, common items, and link items.

Table 13: Tests Used in the Empirical Studies of this Dissertation Project

Inventory	Maximum Points	Total Number of Items	Items Common with CBI	Link items (all tests)
CBI	31	25		7
CBI subtest	25	22	22	7
CBI pre-test	23	22	7	7

CBI

The *Chemical Bonding Inventory* (CBI) is the full inventory with 25 items and a maximum score of 31. The inventory is used to assess students' conceptual understanding and the prevalence of misconception after they have been instructed on the topic of chemical bonding (intermolecular forces included). The full CBI was administered during the *university evaluation study 2, the university intervention study* (at pre-test, re-test, post-test, and follow-up), and in the *Gymnasium intervention study* as a follow-up test. See appendix 1.1 for all items.

CBI subtest

The *CBI subtest* (maximum score of 25) contains all items of the CBI, except for the in-depth evaluation of the understanding of intermolecular forces (items Q23 – Q25). Items common with the CBI (items Q1 – Q22) were developed and optimized in the *Gymnasium piloting phase* and the *university piloting phase*. The CBI subtest was administered during the *university evaluation study 1* and in the *Gymnasium intervention study* at post-test.

CBI pre-test

The *CBI pre-test* is intended to assess prior knowledge of chemical bonding before formal instruction on the topic. Seven items are common with the CBI and CBI subtest, whereas eleven are unique to the test with a maximum score of 23. The CBI pre-test is only used in the *Gymnasium intervention study* as a pre-test. See appendix 1.5 for all items of the CBI pre-test.

3 Promoting the Understanding with Comparing and Contrasting Activities

The evaluation of newly enrolled students' understanding of chemical bonding clearly showed a tendency to overgeneralize the concept of covalent bonding as well as challenges when differentiating between the types of bonding present in substances. The level of understanding of the differences between chemical bonds and intermolecular forces needs improvement also in this highly selective sample of university students. This raises the question of how to foster the understanding of those fundamental chemistry concepts.

Previous investigations on students' understanding of chemical bonds (e.g. Gillespie & Robinson, 2007; Levy Nahum et al., 2010; Othman et al., 2008; Taber, 1998, 2003; Taber & Watts, 2000; Tan & Treagust, 1999; Treagust, 1988), as well as the studies conducted with first-year university students in this dissertation project (see chapter 2), shed more light on the challenges students face when learning about chemical bonds. While more insights into students' difficulties are certainly beneficial, it does not directly provide an answer to the questions of how to overcome those challenges or facilitate learning for students.

As described in chapter 1.1 in more detail, there is a severe lack of concrete methods of how to tackle the challenges. Concrete attempts how to improve students understanding when it comes to learning about chemical bonds are rare. According to a recent review article (Hunter et al., 2022), there are only a handful of investigations conducted until 2020 and none cover the whole topic of chemical bonding or lack in empirical evaluation. Hence alternative ways of how to teach about chemical bonding need consideration. While the identification of the challenges does not directly provide the solution it can still help in guiding us toward it. What have other groups of science education researchers found when it comes to tackling the before-identified main challenge – overgeneralization and the keeping apart of similar concepts? The method of *comparing and contrasting* has shown promise in this regard. But how do learners profit from comparing activities in general and which learning processes are involved?

3.1 Learning by Analogical Processing

Investigations have shown that humans possess the ability to learn by comparison from a very young age. In a series of investigations with infants, Gentner and co-workers could show that small infants could learn about the concept of *same* and *different* by comparing different situations (Anderson et al., 2018; Ferry et al., 2015). In a recent investigation even three-month-old infants were observed showing a longer interest span on object pairs that were different after they were shown two identical items multiple times and the other way around (Anderson et al., 2018). The understanding of such relational information and the following abstraction of such concepts is possible due to the human's unique ability to learn by analogical processing which also sets us apart from other primates (Penn et al., 2008). This means that humans can learn about an abstract relation upon observing multiple events and build categories thereafter to understand the surrounding world (Gentner & Markman, 1997; Markman & Wisniewski, 1997).

With the proposition of the *structure-mapping theory,* Gentner (1983) offered a theoretical framework for potential learning by comparison. The theory describes the process of human comparison as a *structural alignment* of two situations represented in the mind of the learner. This *structural alignment* then leads to the determination of the commonalities and differences between those situations and gives rise to potentially four kinds of learning: *abstraction, difference-detection, inference-projection,* and *rerepresentation (Gentner, 2010)*. *Abstraction* describes the process of extracting the common structure of the observed situations or concepts during the process of repetition of such concepts or tasks. When the compared concepts or situations are different and presented in close temporal proximity the learner's attention is more strongly directed towards the differences between the concepts – describing the process of *contrasting* or *difference-detection*. *Inference projection* describes the process of transfer of the relational structure from one situation to another as can for example be observed when using analogies. *Rerepresentation* occurs when the mental representation of a concept is changed after working with another example or task of such a concept. While the theory of *structural alignment* was originally validated by results stemming from research on category learning, it has a potentially wider range of applications and may serve as a basis for explaining differences in learning gains when investigating the effectiveness of acquiring other and more complex relational information (i.e. mathematical procedures, science concepts or everyday relations) rather than only category learning.

How can we use this information to argue for or against a method of teaching about chemical bonding? Again, we are faced with the challenge of overgeneralization of three similar concepts of bonding. What could be undertaken to better prepare students against using the wrong concepts? One possibility is to change the sequence of when we introduce the different bonding concepts, which concepts we compare, as well as how often we compare and contrast those concepts.

The important point to make is the sequence of how we present such concepts is relevant (Carvalho & Goldstone, 2017). As educators, we have the option to introduce concepts *sequentially* (i.e. *blocked*) or in an *interleaved* manner (Figure 19, top). The sequence influences how we learn and perceive concepts since analogical comparisons can happen inherently. Additionally, we have the possibility to instruct students to actively *compare* concepts. Depending on the level of similarity of the concepts, commonalities or differences are made more strongly salient (Figure 19).

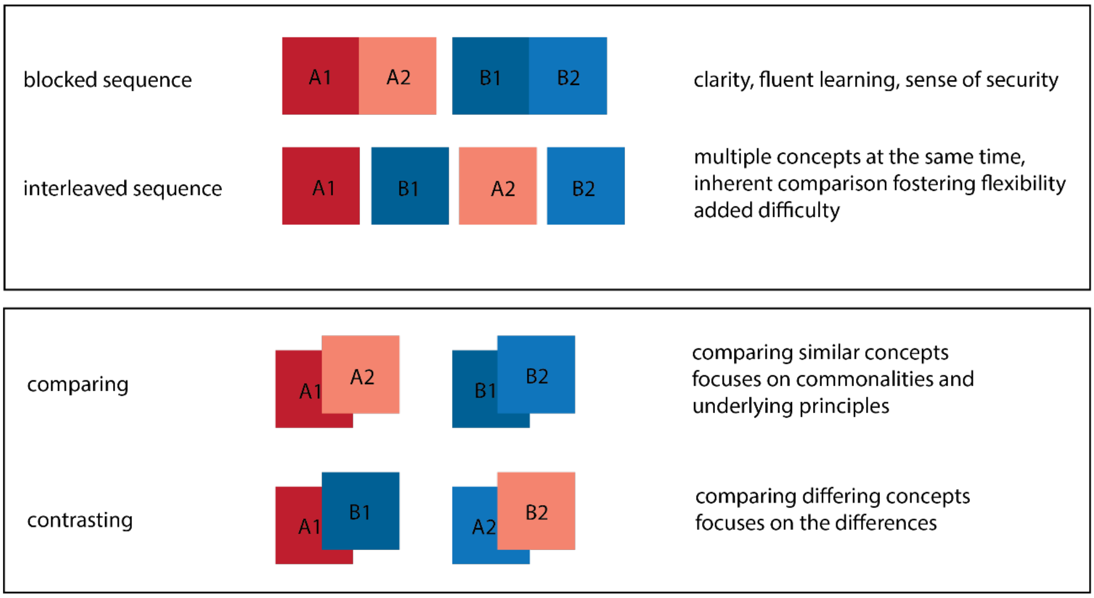


Figure 19: Illustration of different sequencing methods for the introduction of concepts: blocked vs. interleaved (top), introduction by comparison of similar or differing concepts (below). A1 and A2 respectively B1 and B2 are examples of the same concept to be learned.

Blocked and Interleaved Sequencing

A *blocked* sequence of tasks describes a process during which the same concept or principle is encountered multiple times in a row. Before the next concept is introduced, there was enough time to solve exercises that foster the understanding of the first concept or principle. Different principles or concepts are introduced sequentially after each other. This arrangement has the advantage that it will give students a sense of security and promote a feeling of competence. In this setting students usually make few mistakes since they know what concept and principle to use beforehand and students themselves describe their learning as ‘fluent’ (Yan et al., 2016). The common approach to teaching about chemical bonding is in fact to introduce each bonding type after the other, i.e. applying a blocked sequencing.

Interleaving (i.e. applying an interleaved sequence) describes the process when different concepts or principles are used after each other without explicitly comparing the different concepts with each other. With this sequencing method, learners are tasked with solving exercises regarding one concept or principle, and then alternating with that, they have to solve other exercises where another concept is needed. Applying such sequencing will foster flexibility in using different concepts at the same time and also helps to keep different but easy-to-confound concepts apart. Even though students are not tasked with explicit contrasting activities, it can be argued that the process of *contrasting* is still happening inherently. According to the *sequential attention theory* proposed by Carvalho and Goldstone (2017), students will keep previously encountered tasks in mind and inherently make comparisons to the current task at hand. This means that while students are faced with an interleaved sequence of tasks they will be contrasting the different concepts inherently. Since it is not clear from the beginning which concept or principle is to be used, they need to focus their attention on their corresponding mental representation of that concept in their mind. According to Gentner (2010), this will foster learning via *inference-projection* and potentially lead to *rerepresentation* if the mental concepts need adaptation after encountering this new task. According to a meta-analysis conducted by Brunmair and Richter (2019) across all conditions interleaving fosters inductive learning more strongly than blocking (hedges g = 0.42). But it is dependent on the context and very dependent on the concrete learning materials: Investigations with visual learning materials (i.e. naturalistic photographs, paintings, or artificial objects) showed moderate to large beneficial effects for inductive learning of category structures compared to the blocked presentation. When the learning materials were composed of expository texts and tastes, on the other hand, there was no evidence found for a beneficial effect. When the subject to be learned was words, even negative effects of interleaving were observed. The authors caution the readers that there have not been enough studies to conclude concisely that interleaved learning with expository texts, tastes, and words would have no or negative effects compared to the blocked presentation. It is of interest that the authors find stronger advantages for the interleaved condition when the different categories are similar hence easier to confound and with increasing complexity of the content to be learnt.

Comparing Similar or Strongly Differing Concepts

An alternative possibility to introduce concepts is to present students with multiple cases for students to *compare* from and extract the principle themselves. There is a multitude of studies showing that learning from comparing cases can foster the extraction of general concepts or categories more strongly than presenting the contents in a blocked manner (for an overview see Alfieri et al., 2013). Taking into account the theory of *structural alignment* it is very plausible that the process of *abstraction* of a common underlying structure is easier when comparing similar cases. The commonalities and general concept is highlighted and becomes more salient to students (Gentner, 2010). Thereby students gain awareness of the common features of a category (e.g. a certain type of bonding) without implementing the surface characteristics of each case (e.g. whether the substance is solid, liquid, or in a gaseous state at room temperature). Understanding the principle behind a task or concept on a more abstract level is what is usually needed if we desire to foster students' understanding that is transferable to new situations.

When comparing strongly differing cases or concepts students will be drawn to see the differences rather than the similarities. Through the process of *contrasting* educators can focus students' attention on the differences between concepts. It is to be expected that during students' *structural alignment*, *difference-detection* is most strongly pronounced (Gentner, 2010). While strongly differing concepts or categories will inherently induce *difference-detection* it is noteworthy that students might have to be guided in looking for differences rather than similarities explicitly. If we compare ionic and metallic compounds, for example, there are also similarities to find like the ordered arrangement in an ionic respectively metallic lattice or the fact that most ionic, as well as metallic compounds, are present in their solid physical state at room temperature. It becomes clear also from a theoretical point of view that contrasting the different bonding types could be a chance for educators to focus students' attention on the differences between the bonding types. This could potentially reduce students' tendency to overgeneralize the covalent bonding type and make students more strongly aware of the differences between the bonding types.

In conclusion, there are four different possibilities to sequence the introduction to new concepts or principles. While a *blocked* sequence fosters students' feeling of security and fluency during the process of learning, *comparing* activities are especially beneficial for pointing out the commonalities and the abstract structure behind tasks. *Contrasting* activities will foster students' awareness of differences between concepts and *interleaving* of concepts will potentially help students' flexibility to use those different concepts appropriately and distinguish them from each other. Which sequencing method has the potential to tackle the observed difficulties associated with learning about chemical bonds? Looking at it from a theoretical point of view as well as taking into account the empirical evidence gathered in the field of category learning, comparing and contrasting activities show great potential. Interleaving activities that make use of the different bonding types are of potential interest as well.

3.2 Adding Desirable Difficulty

When concepts or principles are introduced in a *sequential* or *blocked* manner, students are less likely to be confused and make mistakes during the process of learning about new concepts. But there is evidence that introducing another concept at the same time or shortly after the first one has been introduced can foster learning more strongly. Due to higher cognitive load, students will struggle more with the task, will describe their learning as less fluent (Yan et al., 2016), and will make more mistakes, but exactly this struggle might be the key to explaining why such sequencing might show advantages in the long-term. While learning is often experienced as more difficult and confusing during the process, it might also be that more reflective processes are induced by such a setting (Carvalho & Goldstone, 2017; Gentner, 2010). Bjork (1994) shaped the term *desirable difficulty* and advocates for training situations to be challenging enough and cautions against removing too many difficulties and obstacles learners might encounter during a process. While adding difficulty for learners might seems counterintuitive to many educators, it might well be the key to a better long-term understanding of some concepts. It must be noted that introducing too many difficulties will add to the cognitive load of the learners – a positive learning outcome can therefore not be predicted beforehand. Since cognitive abilities of learners vary, it remains to be seen whether for some the cognitive load was too much of a challenge and hinder learning more strongly than fostering long-term understanding of a topic.

3.3 Studies on Comparing and Contrasting in Mathematics

As previously mentioned, most of the original research into the sequencing of tasks stems from research on category learning and mathematics (e.g. Rohrer, 2012). But there have been attempts to examine the benefits of case comparisons in classroom settings. Rittle-Johnson and Star's investigation into comparing mathematical problem-solving strategies with fifth- to eighth-grade-students consistently showed benefits in terms of flexibility of use of solving strategies if they knew one of the methods beforehand (Rittle-Johnson & Star, 2007, 2011; Rittle-Johnson et al., 2009). In those investigations, students with comparing and contrasting activities showed greater gains in procedural and conceptual knowledge than students learning about the different methods in a sequential manner. In their research, Rittle-Johnson and Star (2011) found that sufficient prior knowledge of at least one method would lead to more substantial learning gains. Taking into account the *structural alignment theory* (Gentner, 2010) we can further rationalize this finding: Analogical learning is accentuated if one method is already well represented in students' minds and gives more rise to the before-described kinds of learning. Students' familiarity with one concept might also help reduce students' cognitive load.

Ziegler and Stern (2014, 2016) showed in two consecutive studies that students' understanding of the concepts of addition and multiplication benefited strongly from comparing and contrasting activities. While experts can keep algebraic principles for multiplication and addition from each other with relative ease – student novices show more uncertainty in distinguishing those two concepts. The principle of multiplication and addition rules in algebra are usually taught in consecutive order. In contrast to that, Ziegler and Stern (2014) randomly assigned half of the students to self-learning materials where they were simultaneously introduced to the principles and rules involving multiplication and addition of variables. Students were let to compare and contrast the different worked examples. The other half of the class was introduced to the rules of addition and multiplication in consecutive order, i.e. they worked with the same worked examples but different in order. They would first be given the examples for addition and only thereafter be given the examples for multiplication. Both groups were assigned the same amount of time to work with the self-learning materials.

In their second investigation, Stern and Ziegler (2016) investigated whether the same study setup would yield similar results when the teaching method was changed from self-learning materials to direct instruction. In both studies, the compare and contrast groups benefited more from the learning opportunities than the sequential blocked groups. Students from the first group outperformed the latter immediately after the intervention as well as three months later at the delayed post-test. It is noteworthy that the benefit of comparing and contrasting became more pronounced with increasing time: Students from the sequential blocked group would make significantly more mistakes after three months than students exposed to the contrasting activities. The increasing difference between the learning benefits points towards the conclusion that comparing and contrasting activities fostered a more sustainable understanding of the concepts. Taking into account the different methods of teaching in the two studies but the yielding of comparable results, it can be concluded that the type of tasks played a more substantial role than the teaching method (self-learn materials or direct instruction).

These findings could be replicated in a further study conducted by Ziegler and colleagues (Ziegler et al., 2019). The comparing and contrasting activities led to the most stable learning gains and better retention if compared to the sequential introduction of multiplication and addition. It could be further shown that introduction of multiplication, i.e. the concept with less complexity, before addition was beneficiary to students' learning but not on the same level as in the contrasting condition.

To sum up, it could be shown that a simultaneous introduction with a focus on comparing and contrasting activities can be highly beneficiary for sustainable learning of similar concepts, like the algebra rules of addition and multiplication, which are easily confused. Ziegler and colleagues would go on to ask the question, of how students' understanding would profit most from contrasting activities (Ziegler et al., 2018). In this investigation, two groups were simultaneously introduced to the algebra principles of addition and multiplication in a mixed contrasted way, as this has been previously shown beneficiary for learning those concepts (Ziegler & Stern, 2014, 2016). The groups differed in the way students were directed to do comparisons between the two concepts. While there was the *explicit* learning group which would verbalize the differences and the *implicit* learning group which was given more examples to work with and directed to generate new examples. It was to be expected that through extensive problem-solving that students would implicitly derive the underlying differences between the concepts. The interesting finding was, that the common saying "practice makes perfect" might not hold true in all cases: Even though students from the implicit learning group had more opportunities to train with examples they were outperformed by the group that was directed to verbalize the differences with less time left to do exercises. The explicit directive to verbalize the differences lead to greater gains in problem solving skills as well as concept understanding measured three times over a period of ten weeks. In result, there is some evidence that explicit verbalization might help direct students' attention to the difference of two similar concepts more strongly than implicit comparison and repetition.

3.4 The implication of Preexisting Research for the Teaching of Chemical Bonding

Taking into account the above-presented research several possible inferences can be made for designing a teaching unit about the different types of chemical bonds.

With regards to sequencing as well as research stemming mostly from category learning, it became clear that *comparing* and *contrasting* activities bare great potential to direct students' attention toward the differences in bonding types. While it is possible to distinguish between comparing and contrasting on a theoretical level, it is also inherent to analogical processing that there is no *contrasting* without *comparison*. Since the comparisons will inherently be made between the bonding types there are of course similarities as well as differences to be observed. Depending on where the focus is laid we would rather talk about contrasting than comparing or vice versa. Therefore, I will be referring to comparing and contrasting activities often as a pair instead of singling out one. I would even argue that both activities are important to achieve certain learning goals since they differ in activating different types of processes involved in analogical learning (Gentner, 2010).

Interleaving with a focus on the fostering of flexible use of different concepts is of interest as well. It might foster students' ability to differentiate between the bonding types and potentially help students in their choice of which method to use in a certain situation.

Investigations in classroom settings that made use of comparing and contrasting activities are of great promise (Rittle-Johnson & Star, 2011; Rittle-Johnson et al., 2009; Star & Rittle-Johnson, 2009; Ziegler et al., 2018, 2020; Ziegler & Stern, 2014, 2016). They have in common that they were all set in classrooms where mathematical concepts were taught and that comparing and contrasting conditions were efficient in fostering students' understanding and flexibility in using different problem-solving strategies (Rittle-Johnson et al., 2009; Star & Rittle-Johnson, 2009) or algebraic principles (Ziegler et al., 2018; Ziegler & Stern, 2014, 2016) more strongly than in blocked arrangements of concepts. A stronger focus was also laid on the simultaneous introduction of different concepts in comparison to the acquiring of a consecutive introduction. Even though it has not yet been shown that comparing and contrasting activities are beneficial in the field of chemistry education, there is no apparent indication that learning about chemical concepts might not also profit from such activities. The theoretical reasoning behind the advantages stems from general analogical reasoning, and should hence not be domain-specific (Gentner, 2010; Gentner & Markman, 1997; Holyoak & Thagard, 1997).

3.5 Novel Challenges Compared to Existing Studies Involving Comparing and Contrasting

While research on category learning was able to clearly distinguish between blocked, comparing, contrasting, and interleaving conditions, it is a challenge to do so, when the concepts to be taught are of a certain magnitude. This project aims to design a teaching unit about all three bonding types and to give an introduction to intermolecular forces. Following common curricula, this comes with many abilities and competencies students are supposed to be acquiring. Following common practice, chemistry educators will at least spend 25 to 30 lessons on the topics. It is simply impractical, and arguably also not very efficient, to teach so many lessons with the use of only one of the sequencing methods before mentioned. Nevertheless is possible to differ from the typically blocked sequencing and apply a sequence that will be using more of the before mentioned comparing and contrasting activities instead of teaching the different bonding types after each other and only comparing them at the very end. It is also possible to implement interleaved activities in which students need to make use of different types of bonding after they have been introduced to the different concepts.

In Ziegler and Stern's (2014, 2016) studies mathematical principles were introduced simultaneously, and students were prompted to compare the different sets of rules when encountering multiplication and additions of variables. While there are also some principles to be learned when it comes to learning about chemical bonding, there is still a qualitative difference between chemistry and mathematics. I would argue that a concept of a chemical bond is more than a set of rules: Students need to acquire a mental representation of a bonding situation and see the differences between bonding situations. There are many similarities but also differences to be aware of on various levels: e.g. regularity of arrangements of particles, different states of charges (i.e. ions, neutral atoms), and awareness of the formation of stable subunits like molecules. Additionally, we face the complex problem of teaching about something students never observe on the microscopic level but have made experiences within the macroscopic world (Taber, 2013). While the previous studies introduced two different sets of principles at the same time, we attempted to introduce three different bonding types simultaneously. One can argue with added *desirable difficulty* (see chapter 3.2) but there is also the danger of cognitive overload if the students are introduced to a filth of new information at the same time.

What are the direct implications of those differences? As mentioned before, it is not to be expected that analogical learning about chemical bonding is fundamentally different from learning about mathematical principles. Nevertheless, there are still differences with practical implications: Whereas mathematics is taught at least four to five lessons a week chemistry as a regular course at the Swiss Gymnasium usually only takes up two to a maximum of three lessons a week. This directly influences how long an intervention will take. Given that the concepts take a minimum of about 23 lessons to be taught, interventions will have to be conducted over a longer period of time. The insights from previous research as well as novel challenges were taken into account when designing new learning materials about chemical bonding.

4 Development and Description of Teaching Materials based on Comparing and Contrasting

The second overarching goal of this dissertation project was to develop teaching materials to foster the understanding of chemical bonding. This chapter consists of three parts (see Figure 20): First, to make differences to existing teaching materials more salient, I review existing chemistry textbooks used at secondary level 2 and give a short insight into conventional instruction on chemical bonding at Swiss Gymnasiums (Part I, chapter 4.1). I then describe the process of development and optimization of the teaching materials (Part II, chapter 4.2). Chapters 4.3 and the following describe the novel teaching materials based on comparing and contrasting in more detail.

Part I: Conventional Instruction on Chemical Bonding (chapter 4.1)
- Short review of conventional teaching materials for upper secondary school in Switzerland

Part II: Development and Optimization of Novel Teaching Materials (chapter 4.2)
- Process description of development and optimization of teaching materials

Part III: Description of Developed Teaching Materials (chapters 4.3 – 4.8)
- **Overview** of the five main ideas for the teaching materials (chapter 4.3)
- **Detailed Description** of the main ideas with examples (chapters 4.4 – 4.8)

Figure 20: Overview of chapter 4

4.1 Conventional Instruction on Chemical Bonding at Swiss Gymnasiums

To make the novelties and differences of the newly developed teaching materials more salient, I present a short review of *the* most commonly used Gymnasium chemistry textbook in the German-speaking part of Switzerland: *Elemente* (Stieger, 2018). Moreover, I considered another chemistry textbook from the *AKAD series (Bütikofer & Baars, 2020; Bütikofer, 2020)*. In Table 14 the used sequence of topics is given as well as the number of pages dedicated to the topic.

Table 14: Review of Two Commonly Used Chemistry Textbooks at Secondary Level 2 in Switzerland.

Chapter / topic	Number of pages in *Elemente (Stieger, 2018)*	Number of pages in the *AKAD series (Bütikofer & Baars, 2020; Bütikofer, 2020)*
1. Covalent Bonding / Molecular substances	14	37
2. Intermolecular Forces	3	6
3. Metallic Bonding / Metals	7	11
4. Ionic Bonding / Salts	21	20
5. Overview of the bonding types	0	1

In conclusion, both textbooks use the same sequence to introduce the different topics: Covalent bonding is introduced first, then intermolecular forces, followed by metallic bonding, and concluded with ionic bonding. It is noteworthy that the comparison of the different bonding types is not covered at all in *Elemente* while the *AKAD series* makes use of a very short (1-page) comparison of all types of substances.

Conventional Instruction at Swiss Gymnasiums

The lessons assigned to the subject of chemistry vary. Typically students are instructed 2 – 3 lessons a week, 45 minutes each, depending on the canton. Students are taught for 2 – 3 years as a mandatory course and then there is the possibility to set a special focus on chemistry via elective courses (often together with biology).

While chemistry instruction on chemical bonds at the Swiss Gymnasium level is highly differing from educator to educator, there are some commonalities: The different bonds are introduced one after the other in sequential consecutive order and the different bonding situations are typically only compared at the very end. The order of instruction of the bonding types varies: The majority of Gymnasium chemistry teachers follow the sequence used in chemistry textbooks in Switzerland (see Table 14) covalent bonding, intermolecular forces, metallic bonding, ionic bonding, and comparison of all bonding types at the end (see Figure 21). It must be stated that, whereas the majority of chemistry educators make use of the presented order, some start the sequence with ionic instead of covalent bonding.

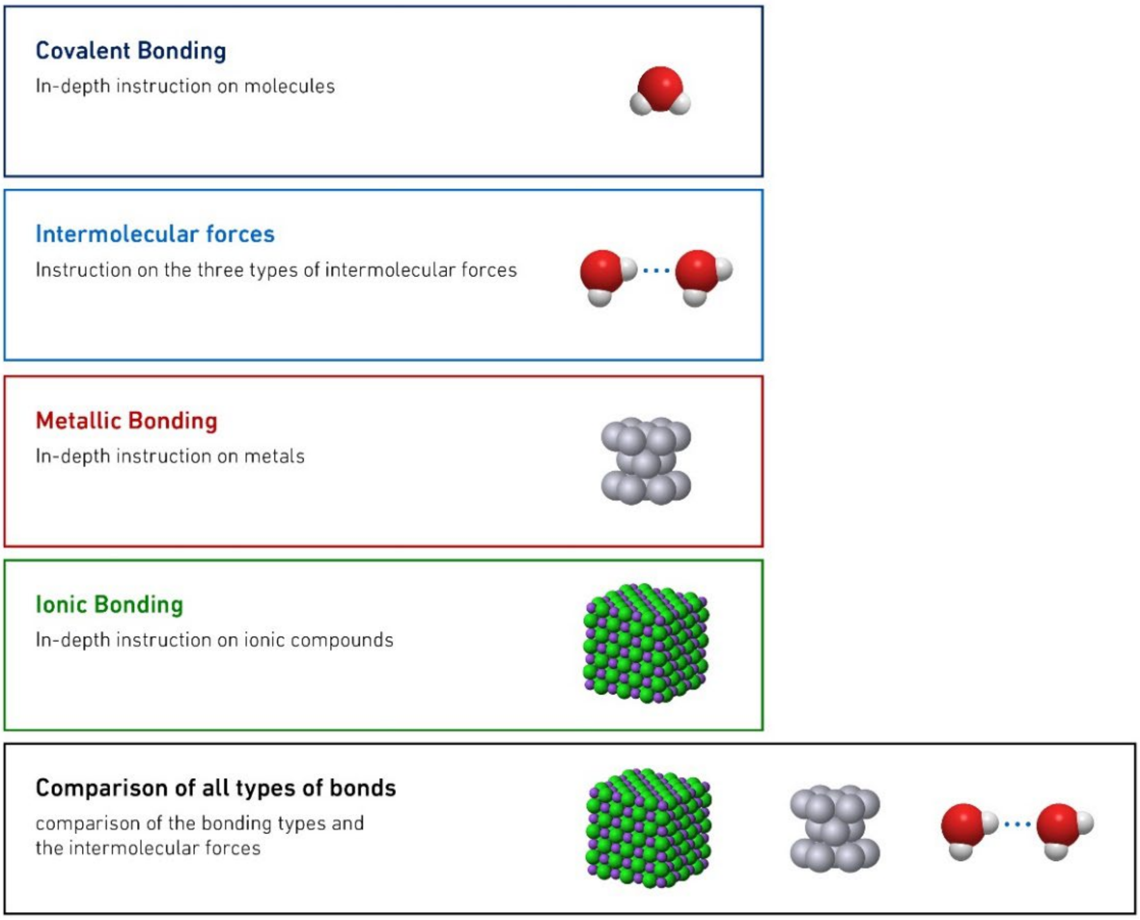


Figure 21: Standard curriculum on chemical bonds: Sequential consecutive instruction on covalent bonds, intermolecular forces, ionic then metallic bonding before comparing all types of bonds.

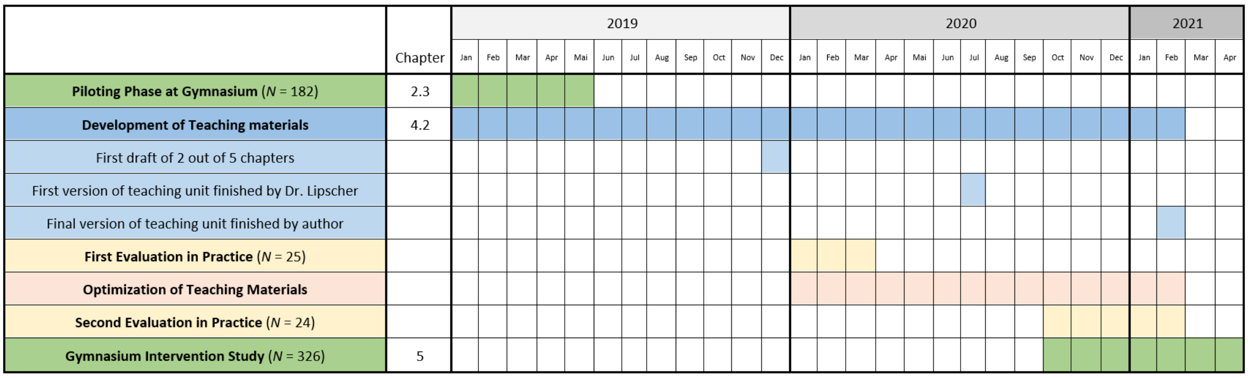
The concept of the covalent bond is normally introduced first. Chemistry teachers will usually do so by introducing the hydrogen molecule (H_2). In the following, students will be taught to use the powerful tool of drawing molecules' Lewis structure. After some practice and discussions about the forces that hold atoms of a molecule together (intramolecular bonds, red in Figure 1, p. 9) teachers will usually go on to talk about intermolecular forces – the forces that occur in between molecules (blue in Figure 1, p. 9).

In the following, metals are introduced, followed by ionic compounds. The nature of ionic bonding is discussed and typical properties of salts are usually part of the standard curriculum. When all types of chemical bonds are discussed, many chemistry teachers do an overall comparison of the chemical bonding situation. This is usually done by assigning different chemical substances to a certain type of bonding and giving typical properties of those substances. The time spent on the different bonding types varies strongly: Typically most of the time is used to discuss molecules and the covalent bond (approx. 7 to 14 lessons). The ionic bonds and the properties of ionic compounds are also discussed in length (approx. 7 to 12 lessons). Metallic bonding is typically only briefly discussed in the standard chemistry curriculum at Swiss Gymnasiums (1 to 3 lessons). The time variance can be explained since some teachers will go into more detail about the properties of the different substance classes (molecules, salts, and metals) directly after they have introduced the bonding type while others will do so at a later stage of the curriculum.

4.2 Development and Optimization of the Novel Teaching Materials Based on Comparing and Contrasting

As described in the previous chapters, one of the main challenges is to teach students how to distinguish between the different kinds of bonds and to foster awareness of the existence of different kinds of bonds. The method of comparing and contrasting has been described as a promising approach for reducing the overgeneralization of similar concepts (see chapter 2.5). Therefore, teaching materials with many comparing and contrasting activities were designed. The goal was to develop and optimize those materials in multiple rounds of teaching and to finally evaluate their effectiveness in comparison to existing teaching material in a classroom intervention study (see chapter 5 for details). See Table 15 for an overview of the Gymnasium studies (in green) the development (blue) and optimization (red and orange) phase of the teaching materials.

Table 15: Overview of the Development (blue) and Optimization Phase (red and orange) of the Teaching Unit.



		2019												2020												2021			
	Chapter	Jan	Feb	Mar	Apr	Mai	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	Mai	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr
Piloting Phase at Gymnasium (*N* = 182)	2.3	🟩	🟩	🟩	🟩	🟩																							
Development of Teaching materials	4.2	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦		
First draft of 2 out of 5 chapters													🟦																
First version of teaching unit finished by Dr. Lipscher																				🟦										
Final version of teaching unit finished by author																											🟦		
First Evaluation in Practice (*N* = 25)														🟨	🟨	🟨													
Optimization of Teaching Materials														🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧	🟧		
Second Evaluation in Practice (*N* = 24)																							🟨	🟨	🟨	🟨	🟨		
Gymnasium Intervention Study (*N* = 326)	5																						🟩	🟩	🟩	🟩	🟩	🟩	🟩

First Draft

The teaching materials were designed in cooperation with the MINT Learning Center of ETH Zurich under the supervision of Dr. Ralph Schumacher and Prof. Dr. Andreas Vaterlaus. At the MINT Learning Center, science teachers are developing teaching materials containing many tasks with learning methods that have proven empirically effective and cognitively activating. *MINT* stands for mathematics, informatics, natural sciences, and technical sciences, equivalent to the English *STEM* term.

The basis for the teaching unit was laid by a team of cognitive science and education researchers as well as chemistry practitioners: Dr. Juraj Lipscher, with his 35 years of experience as a chemistry teacher on the Gymnasium level and author of three other teaching units at the MINT Learning Center, Dr. Ralph Schumacher cognitive scientist and researcher at the MINT Learning Center and the author with a background as a chemist and limited experience as a chemistry teacher. Additionally, I could count on the expertise of Prof. Dr. Antonio Togni for advice on detailed knowledge in the field of chemistry. The expertise of Prof. Dr. Elsbeth Stern had proven very useful for the design of the questionnaire, the choosing of the appropriate methods, and the overall study design.

The development of the teaching materials for the topic of chemical bonds started in early 2019. At the time I was conducting the first assessments of students' understanding of chemical bonds at the Gymnasium level (see chapter 2). The first conclusions from those studies as well as my research into previously described misconceptions in literature influenced the development of the teaching materials substantially. While the lead for the design and writing of the first draft was in the hand of Dr. Lipscher, we held many discussions on how to best proceed with the teaching unit. A first draft of the first chapters (introduction and parts of the ionic bonding chapter) was available in December 2019.

First Evaluation in Practice

In January 2020, I was offered the opportunity to evaluate the practicality of the so-far-developed teaching materials at the Gymnasium Oerlikon Nord (Zurich, Switzerland). I was able to use the developed teaching materials and teach 24 lessons on chemical bonding in a class of 25 10th graders (mean age of 17). Even though the first two chapters of the teaching unit had been written, they were not yet planned in detail as individual lessons. I, therefore, discussed the lessons beforehand with one to two experienced chemistry teachers at the Gymnasium. The combined expertise was used to take the first draft of the teaching materials and structure the content such that it would fit into 45-minute lessons. A special emphasis was laid on the introduction of the lessons: To assure an appropriate cognitive activation at the beginning of each of the lessons, I had to come up with additional introductions and additional experiments. Since the chapters on metallic and covalent bonding were not yet finished at the time of the teaching, I designed new worksheets and teaching materials shortly before I had to teach them.

Unfortunately, the breakout of the COVID-19-Pandemic brought the first evaluation phase to an unexpected halt, since teaching in class was no longer a possibility after mid-March 2020. At that point, I was not yet able to finish my instruction on the topic of covalent bonds. The evaluation of students' understanding of chemical bonding was planned as a pen-and-paper questionnaire after the instruction. At this stage of the project, an online version was not available and could therefore also not be used. The topic of chemical bonds wasn't completely taught and there were many external factors due to the pandemic that could have influenced the outcome of such an evaluation. When the students finally returned to the classroom too much time had passed already. I, therefore, decided against an in-depth analysis of students' learning gains.

In general, one could conclude that the use of the teaching materials and the first adaptation in the school setting was successful. Even though students were exposed to a more challenging introduction with three different bonding types and intermolecular forces they were generally able to follow my instruction. Of course, as is typical for the first-time application of new teaching materials, there was room for improvement. Nonetheless, this first evaluation phase was encouraging since it showed that the chosen approach is generally applicable in a regular school setting.

By the summer of 2020, Dr. Lipscher had finished the chapter on metals, covalent bonds, and a chapter on the properties of different substances. Dr. Lipscher would enjoy his retirement after having finished the first draft of the teaching materials that built the basis for these teaching materials. The implementation of some of the new ideas, worksheets, tasks, and changes that were deemed necessary after having taught the lessons would fall into my domain from then on.

Optimization of the Teaching Materials for the Second Evaluation in Practice

Whereas one could say that it was possible to introduce three bonding types simultaneously, it became also clear that the level of detail during this introduction phase is crucial. In the first evaluation phase, six lessons were used to introduce the different bonding types in quite some detail. For substances containing covalent bonds, there are three bonding possibilities to constitute substances: small molecules, larger molecules up to huge molecules like DNA, and diamond-like substances. Following our first draft, I taught about them in the introduction chapter. Additionally, I introduced the intermolecular forces in a general manner at that point. From a retro perspective, this was deemed inefficient. The detailed introduction gave rise to repetition since the bonding types were discussed in the following lessons in more detail anyways. While it would be desirable on a theoretical level that students have an understanding and awareness of all bonding possibilities in detail as well the intermolecular forces from the beginning, it became also clear that this would not foster students' understanding in a way that they obtained a good overview of the possible bonding situations in substances. Therefore we decided to shorten the introduction to focus students' attention on the most important facts:

- There are three bonding types.
- *Electronegativit*y is the relevant concept to explain differences in bonding situations between atoms.
- The type of bond can be assessed by evaluation of the types of atoms substances contain (metals and or non-metals).

Therefore, the major adjustments for the introduction were the following:

- The introduction was shortened to fit into two lessons. Giving only an overview of the three major bonding situations, neglecting the intermolecular forces at the very beginning.
- Stronger emphasis on the three bonding types using colors in the overview map.
- Simplification of the overview map by omitting high molecular weight substances and diamond-like materials at the beginning.

Second Evaluation in Practice

In October 2020 the optimized teaching materials could be evaluated and optimized in a school setting for the second time. I organized to teach another class of 24 10th graders (mean age of 17) at the Gymnasium Hohe Promenade in Zurich, Switzerland. As every educator would probably agree, newly developed teaching materials typically profit immensely from the second round of teaching and optimization. I used the first evaluation phase to mainly evaluate the general feasibility of a simultaneous introduction of all bonding types. This second evaluation aimed to see whether the made adjustments and new ideas that I implemented after the first evaluation phase would foster students' understanding even better.

The second evaluation round was also the start of the *Gymnasium intervention study* (see chapter 5 for details). I was teaching three lessons a week and always preparing the lessons beforehand. At the same time, I had feedback from three other chemistry teachers involved in my intervention study. They were teaching with the developed teaching materials with a delay of a few weeks. On average, I led a discussion of one hour with each of the teachers every week. In those discussions, they also gave feedback on the classroom practicality of the teaching materials. Some of the discussions also led to improvements and adjustments. This mechanism also provided for feedback to identify subtopics that were seen as central to the topic of chemical bonding on the Gymnasium level. Whereas I implemented some of them, others were deemed to be more of an in-depth topic that could also be discussed in class after the end of the intervention. The aim to only implement what the majority of chemistry teachers would deem as necessary to teach was reached since no teacher so far claimed that the teaching materials cover topics that they do not cover in class as well.

The teaching of the shortened version of the introduction was a success. The simplification and abstraction of the most important points were successful: Students got the basic idea of the existence of three bonding types at the very beginning. The details of how those bonding types would lead to different bonding situations in substances, i.e. substance classes, were easily understandable when the individual bonding types were discussed in more detail. The teachers made acquainted with the teaching materials found that the teaching materials were generally “interesting and applicable” and an “interesting alternative to the common way of how the topic was taught”. While the optimization process of teaching material is still ongoing, this final version sets high standards for teaching material on chemical bonding. The teaching materials can readily be used on the Gymnasium level as has been shown by ten different chemistry teachers so far.

4.3 Five Main Ideas and Novelties of the Teaching Materials Based on Comparing and Contrasting

This section aims to give a brief overview of the *five main ideas* (1 to 5 below) that shaped this teaching unit and the most important implementations made, before describing each of the five main ideas in more detail in chapters 4.4 – 4.8.

1. Fostering Students' Awareness of the Existence of Three Bonding Types
(for more details, see chapter 4.4)

"There are three types of chemical bonds (with equal relevance for daily life)."

- Sequencing of topics: simultaneous introduction of all three bonding types, followed by an in-depth study of ionic bonding, metallic bonding, and covalent bonding, closing with an introduction on intermolecular forces
- Early introduction of the concept of electronegativity to rationalize differences between bonding types (usually only introduced for polar covalent bonds)
- Use of a memorable analogy (electron thieves and victims) to differentiate between different bonding types and make the concept of electronegativity more accessible.
- Overview graphic of all three bonding types and how to differentiate between those in the sense of a grand roadmap.

2. Fostering Students' Awareness of the Differences between the Different Types of Chemical Bonds (for more details, see chapter 4.5)

"There are major differences between the bonding types."

- Compare and contrast as often and as early in the curriculum as possible: There are 27 learning activities with comparing and or contrasting character in this teaching unit.
- Reoccurring conductivity experiment at the start of the in-depth instruction for each bonding type: The experiment induces the awareness that known bonding concepts do not explain the new observed situation. This new class of substance has different properties due to the new type of bonding present in this substance – therefore using the overview graphic for all bonding types.
- Back referencing to other bonding situations where opportunities arise to do so: e.g. Comparison of ductility of metals and ionic compounds, the difference between polyatomic ions and molecules, integration of salts when drawing Lewis structures of molecules, introductory comparison of a diamond, ice, and sodium chloride crystal, pre-structured concept map of the three bonding types.

3. Fostering Students' Understanding of the Cohesion of Atoms and Ions to Form Ensembles (for more details, see chapter 4.6)

"The strength and the reason behind the attraction of atoms and ions to form ensembles (metals, ionic compounds, and molecules) can be rationalized."

- Coulomb's Law is used as a basis for explaining all of the cohesion forces.
- A level-appropriate model for each bonding type is presented: The model rationalized why atoms respectively ions hold together to form ensembles (ionic compounds, metals, and molecules).
- Different electronegativity values for elements are explained using Coulomb's law, hence making them more accessible to students.
- Heuristics are indicated as such and further rationalized: The noble gas rule is rationalized by explaining why full or empty shells are often encountered in ions by using Coulomb's Law. The application of the noble gas rule in the context of covalent bonding is introduced as a heuristic due to the repulsive forces of doubly occupied electron clouds, i.e. there is no more spatial space than for four doubly occupied electron clouds.
- Giving students a sense of the quantum mechanics theory: Quantum mechanical calculations are also based on Coulomb's Law. Students should learn that their intuitive ideas using Coulomb's law are a good basis for understanding the covalent bonding situation. This is done using the electron probability density of hydrogen as well as a train analogy for the attraction of two hydrogen atoms.

4. Fostering Students' Awareness of the Differences between Intermolecular Forces and Chemical Bonds (for more details, see chapter 4.7)

"Intermolecular forces are only present in molecular substances and their individual strength is smaller by several orders of magnitude compared to chemical bonds."

- Explicit comparison of the relative strength of intermolecular forces with chemical bonds: The relative strength of the different kinds of intermolecular forces is introduced while still keeping in mind that the cohesion forces of chemical bonds are greater by several orders of magnitude.
- Highlighting that intermolecular forces do not occur in metals or ionic compounds.

5. Fostering the Correct Usage of Chemical Bonding Language and the Targeting of Specific Misconceptions (for more details, see chapter 4.8)

"Correct use of chemical bonding language: Refinement of the molecule term, the information content of chemical formula, meaning behind metallic and ionic lattices."

- Refinement of terms used in daily language: The definition of the term "molecule" is sharpened with concrete examples.
- Chemical formula and its information content: Chemical formulas have similarities but depending on the bonding situation present in a substance different inferences can be made. Explicit contrasting of that fact is expected to make the differences more salient to students.
- Targeting observed misconceptions through self-explanations (six times) and holistic mental model confrontation (one time).

Main Differences to Conventional Teaching Materials

What are the major differences between these novel teaching materials compared to conventional teaching materials?

1. Simultaneous Introduction of all Types of Bonds before Going into more Detail

Conventional instruction on chemical bonding is sequential: The different types of bonds are introduced one after the other. This teaching unit introduces all types of bonds at the very beginning in a two-lesson introduction chapter (see chapter 4.4 for more details and the specific realization of the chapter).

2. The Sequencing of Introduction of the Different Bonding Types

While conventional teaching materials introduce the covalent bond first (see Figure 21, p. 66), this unit introduces all types at the same time. Next, the ionic bonding situation is discussed in more detail before going into more detail about metals and covering the covalent bond and intermolecular forces last (see Figure 22, p. 76 for an overview).

3. More Comparing and Contrasting Activities

This teaching unit makes extensive use of the method of comparing and contrasting. While standard chemistry textbooks do not offer any comparison of different bonding types, some teachers compare the different bonding situations at the very end. In this teaching unit, the different bonding types are compared and contrasted with each other all the time from the beginning until the end of the unit.

4.4 Fostering Students' Awareness of the Existence of Three Bonding Types

The evaluations of first-year students' understanding of chemical bonds brought to light that the seemingly simple fact that *(1) "there are three types of chemical bonds"* has not been incorporated into students' minds strongly enough in many cases. However, what could be done to foster students' awareness of the existence of three bonding types? I present teaching materials and new approaches that have been inspired by results from other fields of education research (for details see chapter 3), the experience of chemistry educators, and novel ideas of the authors of this teaching unit. To foster students' awareness of the existence of the three bonding types five new approaches are presented in more detail in the following sections:

1. Simultaneous introduction and order of in-depth discussion of the different bonding types
2. Making students aware of the fact that atoms are held together by forces of different strengths
3. Early introduction of the concept of electronegativity
4. Use of a memorable analogy for the differentiation between bonding types
5. Overview Graphic as a roadmap for learning about chemical bonds

Simultaneous Introduction and Order of In-Depth Discussion of the Different Bonding Types

In this teaching unit, the three bonding types are introduced at the same time (for reasons see chapter 3). This varies strongly from the standard curriculum and is one of the major differences compared to conventional instruction on the topic. Whereas conventional teaching typically use a sequential consecutive order, i.e. in a blocked sequence, I present a method by which the three different bonding types are introduced at the same time. An overview of the structure of the complete teaching unit is given in Figure 22. The simultaneous introduction of three bonding types occurs in the first chapter of the comparing and contrasting teaching unit (Overview, black in Figure 22) and takes up about two lessons.

The other major adjustment is the arrangement of the following in-depth discussions of the topics. As has been established the covalent bonding situation of substances is often seen as *the* model for a chemical bond and many of its associated characteristics (e.g. the composition in small molecules and intermolecular forces in-between such molecules) are hence wrongly believed to be valid for the ionic and metallic bond. After a brief introduction to all types of chemical bonds, the type that is first discussed in more detail is the ionic bond (green in Figure 22), followed by the metallic bonding situation (red). The covalent bond and intermolecular forces (blue) are discussed last to break its typical dominance in many of the students' mental representations of chemical bonds.

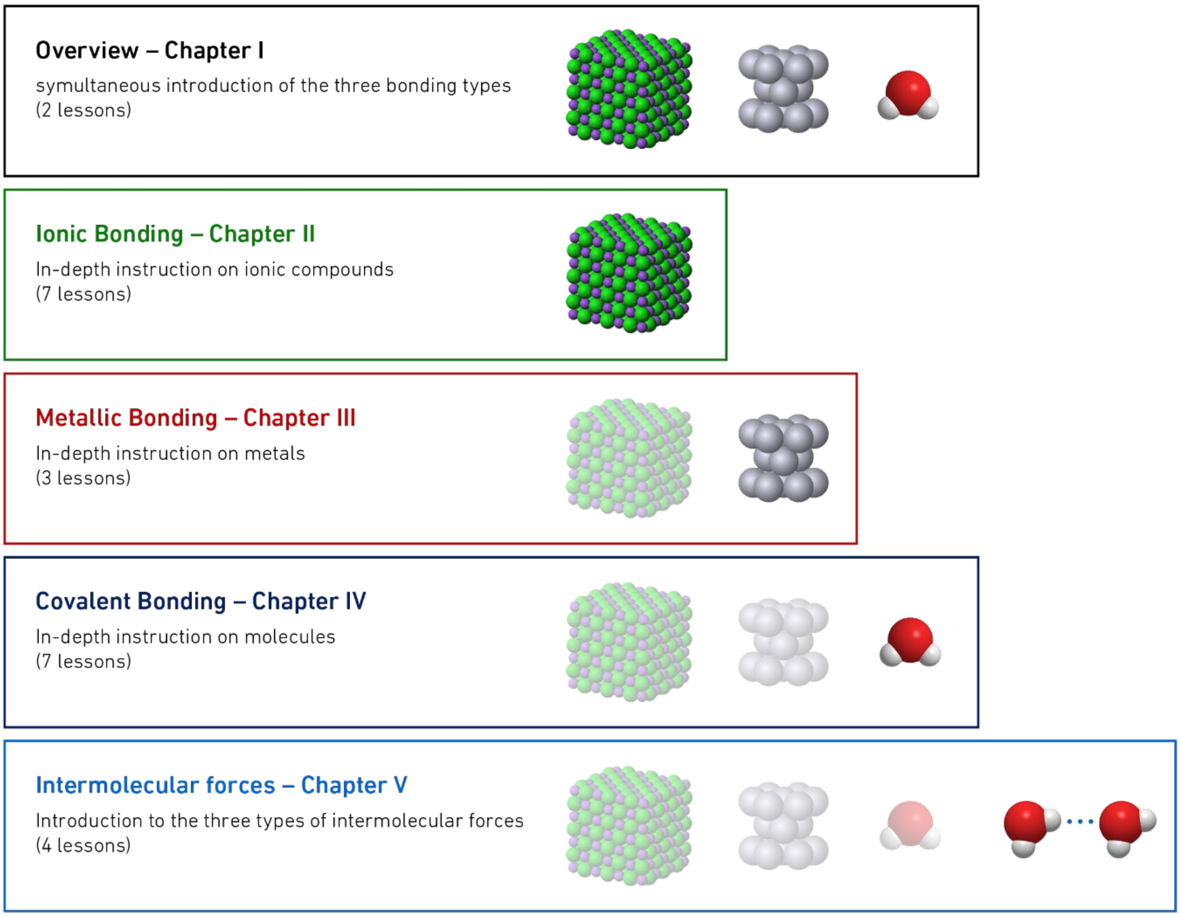


Figure 22: Overview of the structure of the developed teaching unit: The three chemical bonds are simultaneously introduced in an introduction chapter I, followed by an in-depth discussion of ionic compounds, then metallic bonding and covalent bonding. Students are kept aware of the other so far covered existing bonding types while learning about the new type of bond in more detail.

Making Students Aware of the Fact that Atoms are Held Together by Forces of Different Strengths

As chemistry experts, we take the fact for granted that there are chemical bonds holding atoms together. We also know that there are three kinds of bonds which result in macroscopic observable differences of substances containing certain kinds of bonds. For students, this is everything but obvious. Students can go through their daily life without ever asking themselves the question of why substances possess different melting points – even when they are aware of the fact that not all substances are in different physical states (e.g. water is liquid at room temperature and melts at 0 °C while a solid candle must be heated up to become liquid). So how can we make students see those differences? The introduction of this teaching unit, therefore, makes them aware of the fact that there are differences we need to be able to explain. To make this fact more salient, students are confronted with three substances they know from daily life with similar surface characteristics but strong differences in their melting points (. Students are prompted for about five minutes to make educated guesses for the reason behind the differences in melting points and their similar appearances.

Water / Ice	**Sodium chloride**	**Diamond**
H_2O	NaCl	C
		
Melting points		
0 °C	801 °C	about 4 000 °C

Question: How is it possible that substances that look so similar have such different properties? Consider the similarities and differences of these substances at the subatomic level (i.e. particles and bonds). Could they explain the similarities and differences between the substances?

Figure 23: Introductory task of the teaching unit (see appendix 3 worksheet I/1): Students are prompted to make educated guesses on the reason behind de differences in melting points of ice, sodium chloride, and diamond (Rob Lavinsky, n.d.).

Students are supported with two follow-up questions:

- What structural features could be responsible for the similar appearance?
- And what relationships between the particles could be used to explain the differences in the melting points?

This introduction has the advantage to activate students' prior knowledge, making students think about the problem at hand and hopefully become aware of the limitation of their knowledge. Students have not yet acquired the needed concepts (i.e. chemical bonds, intermolecular forces) to explain the observations. The students are told that at the very end of the teaching unit an appropriate explanation for those three substances will be given (see next section, p. 95). Nevertheless, some inferences should become clearer for students after this introduction:

1. There are forces that hold atoms or particles together (e.g. chemical bonds – the topic at hand)
2. There are big differences in the strength of this cohesion.
3. We cannot directly deduce inferences by simply looking at surface characteristics.
4. Metacognition: The known concept (particle theory) is not sufficient to explain the differences.

Early Introduction of the Concept of Electronegativity

The introductory task sets the stage for the introduction of the concept of electronegativity. Students' lack of a concept to rationalize the huge differences in strength of attraction can be used to confront them with the question: Why do attracting forces even exist? Atoms possess the same amount of protons and electrons, i.e. the same amount of positive and negative charges, resulting in a net neutral charge. Following Coulomb's law, an attractive force between atoms should not exist at all. However, this cannot be, since we all know that the world is not only comprised of single atoms. Therefore, some kind of attractive interaction must exist. When looking at two approaching atoms in more detail (Figure 24) the reason behind the existence of attracting forces can be given in a level-appropriate manner: While the atoms are net neutral the atoms consist of positive and negative moieties. When the distance between two molecules is small enough, those charges play a vital role: While the electrons are attracted to their own positively charged nucleus, attractive interactions with the positive nucleus of an approaching atom are possible as well. This additional interaction is the reason for the building of chemical bonds.

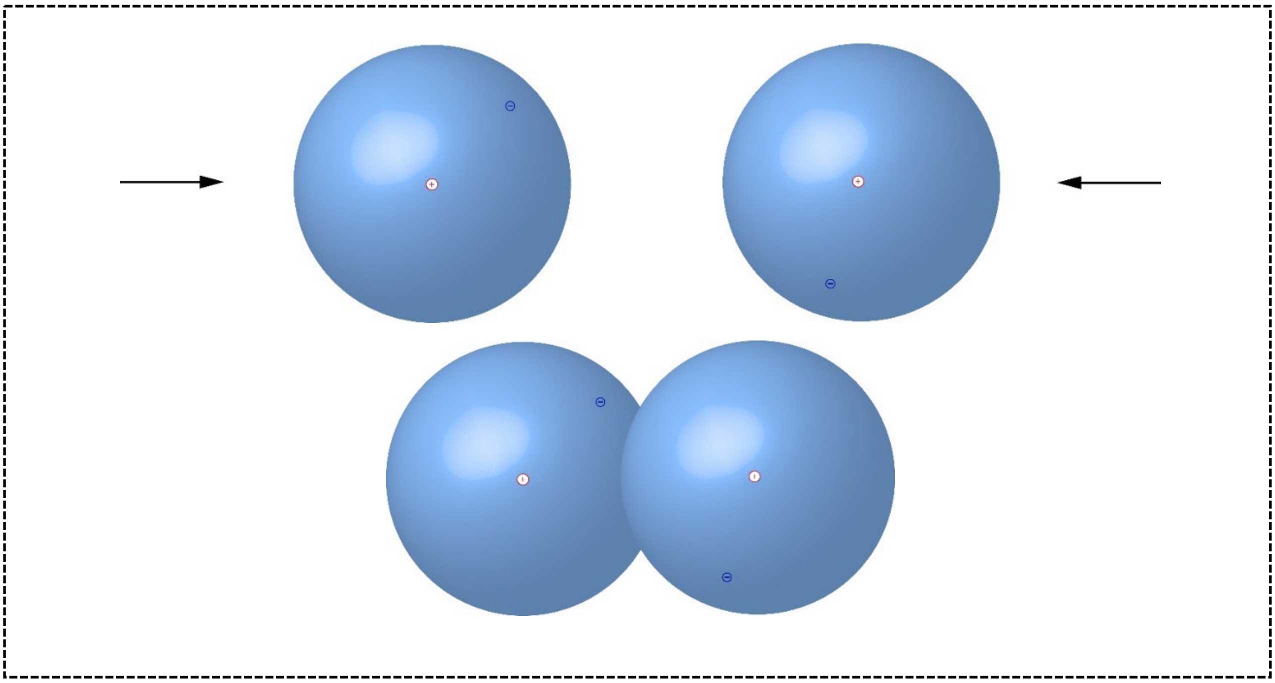


Figure 24: Illustration of two approaching atoms

This does not yet explain why there are such differences between the strengths of different interacting atoms. The concept of electronegativity helps students understand where such differences stem from. To understand how individual atoms can form bonds with other atoms, it is essential to know how strongly an atom can attract not only its own electrons but also the electrons of other atoms (Figure 25).

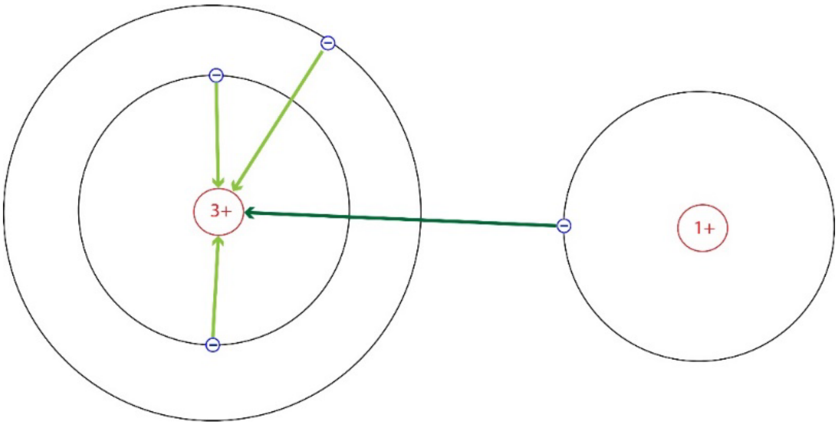


Figure 25: Visual representation of how an atom attracts its own electrons (light green) as well as the electrons of another atom (dark green).

When we compare atoms of different elements, we get a relative measure of a property called electronegativity, a concept first introduced in 1932 by Linus Pauling. The concept of electronegativity is not usually introduced at the very beginning of the topic of chemical bonds. Wheras, it is *the* essential concept for this teaching unit to distinguish the three types of chemical bonds, normally the concept is used to describe the polarity of covalent bonds. This means that the concept is introduced when talking about intermolecular forces. In many textbooks, the definition of electronegativity then more specific and tailored to fit the narrative to explain differences in the polarity of covalent bonds: Encyclopedia Britannica for example defines electronegativity as “the ability of an atom to attract to itself an electron pair shared with another atom in a chemical bond”. (Encyclopaedia, 2011)
This teaching unit uses the concept in a more general and applicable way hence the definition is the following: *“Electronegativity is a relative measure of how strongly electrons are attracted to an atom.”*

After receiving introductory information about the concept of electronegativity, students have the opportunity to deepen their understanding of how electronegativity is related to the core charge and size of the atoms of different elements. This is done by utilizing the method of *inventing with contrasting cases* that has first been described in the literature by Schwartz and co-workers (Schwartz et al., 2011). The results have been supported by further studies (Kuo & Wieman, 2016; Schalk et al., 2018; Weaver et al., 2018). The method takes advantage of the *difference-detection* and *abstraction* processes that are activated while comparing (Gentner, 2010). Students are asked to compare different cases and therefore deduce the underlying principle, supported by prompts and questions. The comparison of three cases (Task 1, see Figure 26) and the follow-up questions (Task 2 to 5, see Figure 27) help students to make the comparisons of the relevant cases and make the most important inferences based on the coulomb law.

Task 1: Calculate the core charge of a lithium and chlorine atom and enter the number of valence electrons in the following table.

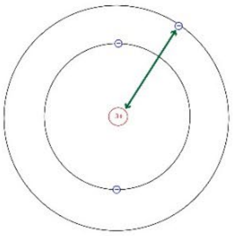
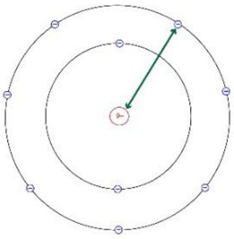
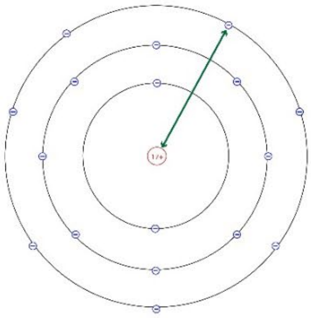
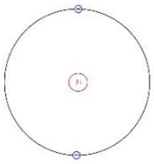
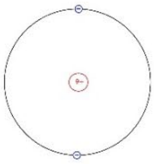
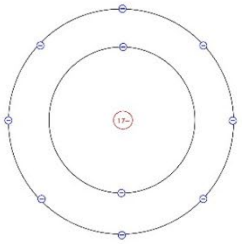
	lithium atom	fluorine atome	chlorine atom
neutral atoms in shell modell			
atomic core			
core charge	1+	7+	7+
valence electrons	1	7	7
electronegativity	1.0	4.0	3.2

Figure 26: Inventing with contrasting cases task to deduce the underlying principle according to which electronegativity values are set. The solutions are given in green.

Task 2: Formulate a simple rule that allows us to find the core charge of any element.

Task 3: A lithium atom has a lower electronegativity value (1.0) than a fluorine atom (4.0). Use the Coulomb law to explain why a fluorine atom attracts electrons more strongly.

Task 4: Chlorine and fluorine atoms have the same core charge, yet chlorine atoms have a lower electronegativity. Can you explain this with the Coulomb law?

Task 5: In the periodic table the electronegativity increases from left to right and decreases from top to bottom. Can you explain this with the Coulomb law?

Figure 27: Follow-up tasks to direct students' attention to the relevant comparisons to be made.

When dividing all the elements into two groups of metals and non-metals, students should realize that metals typically possess low and non-metallic elements high electronegativity values (Task 6, see Figure 28). Task 7 prompts students to come up with the fact that there are only three possibilities to combine those two groups:

1. non-metal and metal (ionic bond)
2. metal and metal (metallic bond)
3. non-metal and non-metal (covalent bond)

Task 6: Consider where metallic and non-metallic elements are located on the periodic table and try to make a rule of thumb regarding their electronegativity values.

Non-metals usually have high electronegativity values.

Metals tend to have low electronegativity values.

Task 7: For the attractive forces prevailing in a substance, it is important whether atoms with low electronegativity (typically metallic atoms) and/or those with high electronegativity values (non-metallic atoms) are contained. What are the possible combinations between the two groups “metals” and “non-metals”?

1. Non-metal + Metal
2. Metal + Metal
3. Non-metal + Non-metal

Figure 28: Task to derive the fundamental conclusion that there are three possible combinations of the two groups metals and non-metals.

Usage of a Memorable Analogy for the Differentiation between Bonding Types

Analogies as an instructional tool for teachers have long been recommended (Gee, 1978; Schustack & Anderson, 1979; Webb, 1985; Weller, 1970). Skilled teachers are still expected to use analogies to support students' learning of new concepts by drawing parallels to examples or concepts they are more familiar with as of today (Buehl, 2017; Richland et al., 2007; Treagust et al., 1992). The basis for such recommendations lies in the vast research literature that has shown analogies' potential in supporting learning, giving explanations, and problem-solving (Council, 2000). Research has for example shown that analogies help students to focus their attention more strongly on key features when encountering new information (e.g. Christie & Gentner, 2010; Gick & Holyoak, 1983; Loewenstein et al., 2003). Hence, analogies can be used as powerful tools for learning and remembering new concepts. Therefore a memorable analogy is introduced to students for the concept of electronegativity and the differentiation between different bonding situations. The following analogy has been brought to my attention by Dr. Juraj Lipscher and Roger Deuber who were using this analogy in their classroom for some years. When dividing the elements of the periodic table into two groups, we find that non-metallic elements generally possess high and metallic elements low electronegativity values. This fact is used to assign titles to those two groups: Electron thieves (non-metals) and electron victims (metals). Electron thieves, like for example a chlorine atom (Figure 29; blue), will detach an electron from atoms with lower electronegativity values (e.g. a sodium atom, red in Figure 29).

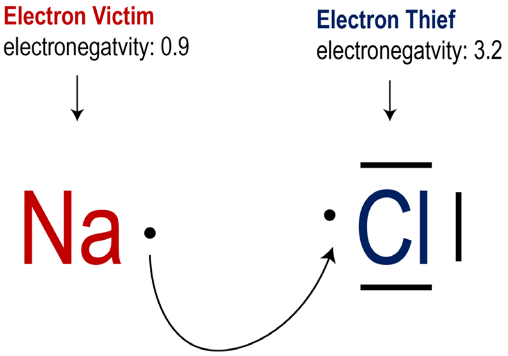


Figure 29: Illustration for the analogy of electron thieves (non-metals) and electron victims (non-metals). The chlorine atom (blue) with higher electronegativity will detach or "steal" an electron from atoms with lower electronegativity like a sodium atom (red).

Why is this analogy so fruitful? Students are very familiar with the concept of thieves and victims. Students already know the concept of stealing and fending off intruders to defend property. In this analogy, electrons are the valued belonging and electronegativity represents the tendency to steal and or the ability to protect their belonging against other thieves (Table 16).

Table 16: Electron Thief and Electron Victim Analogy and the Corresponding Aspects of the Scientific Concept

Aspect of scientific concept	Representation in analogy
Electrons	Valued belonging
Electronegativity	Tendency and wits to steal and ability to protect property
High electronegativity	Electron thief
Low electronegativity	Electron victim

Many chemistry teachers use the ‘noble gas rule’ as an easy-to-remember heuristic to convey to students that some elements end up with more or fewer electrons than their neutral state when looking at typical ions in an ionic compound for example. As long as the rule is introduced as a heuristic that is not problematic. Unfortunately, students are exposed to a lot of online media where the noble gas rule is not used and branded as a heuristic rule but used as a way of explaining *why* electrons are taken up or given away freely. Explanations like “metals like to give away their electrons” or “non-metals take up electrons to achieve the electronic configuration of noble gases” are typical for such explanations. The first statement is simply scientifically wrong: The first ionization energy of metallic atoms is positive since energy must be devoted to counteracting the attracting forces between the nucleus and the valence electrons. Sodium’s first ionization energy for example is 496 kJ/mol (Kaufman & Trowbridge, 1999) and well above zero. With this analogy, students are made aware of the fact that metallic elements do not “want to give away” their electrons freely since they are called “victims” and nobody wants to be a victim. Of course, it is true that when there is a stronger electron thief (i.e. an atom of an element with high electronegativity) the sodium atom will not be able to avert the theft.

The analogy is the basis for the students to understand the different interactions, i.e. different bond types, that can occur if different types of elements (metals and/or non-metals) are combined in a substance:

1. *Ionic Bond:* Electron Victim (metal) and Electron Thief (non-metals)

2. *Metallic Bond:* Electron Victims (metals) among themselves

3. *Covalent Bond*: Electron Thieves (non-metals) among themselves

In the following a shortened version is given, of how the analogy is used to describe the different bonding situations:

1. Ionic Bond: Electron Victim (metal) and Electron Thief (non-metals)

If a thief encounters a victim, it is relatively easy to predict what would happen: The thief will steal the victim’s belongings and become richer. When an element that behaves as an electron thief (non-metal) encounters another element that behaves as an electron victim (metal), the outcome is very similar: The non-metal steals the valence electrons of the metal. Figure 30 illustrates this transfer of electrons from the metal to the non-metal leads to the formation of two ions: one positively charged (metal) and one negatively charged (non-metal):

Figure 30: The electron thief (chlorine atom)) steals an electron from the electron victim (sodium atom resulting in the formation of positively and negatively charged ions.

Ions formed this way arrange themselves in such a way that oppositely charged ions come as close as possible to each other. This cohesion of oppositely charged ions by electrostatic attraction is called ionic bonding. It is very important to emphasize that this process typically happens not only between two atoms, i.e. one electron thief and one electron victim but between many atoms at the same time. This leads to the fact that we not only get one ion pair but a large compound of ions.

2. Metallic Bond: Electron Victims (metals) among themselves

If two or more electron victims meet each other, none of them can defend their valence electrons very strongly, but they will not fight each other over their possessions either. Since they do not have a strong interest in goods, they will rather form a community in which they share their belongings.

Metallic atoms also form huge atomic bonds, similar to what we have seen in ionic bonds. However, since they do not attract their electrons very strongly, the atoms lose their electrons, and then the positively charged core of the atom remains. For this reason, the electrons in a metallic bond are not localized between two atoms as they are in a covalent bond. Rather, they are distributed throughout the atomic bond and are common to all atoms. Such freely moving electrons are called electron gas. The metallic bond thus consists of the attraction between the positively charged atomic cores and the electron gas. Since the attraction between atomic cores and the electron gas is an interaction, it can also be described as the electrons attracting the atomic cores. In this way, it can be said that the negatively charged electron gas holds the positively charged atomic cores together.

3. Covalent Bond: Electron Thieves (non-metals) among themselves

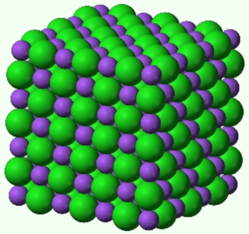
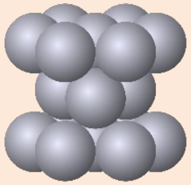
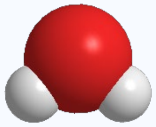
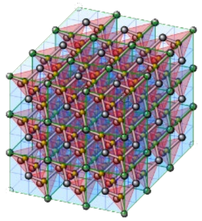
If two or more thieves of equal strength meet, they cannot dispute each other's prey but must divide it between themselves. For example, if two chlorine atoms combine, both atomic nuclei attract the valence electrons of both atoms. This attraction of valence electrons by both nuclei causes the atoms to remain a small distance apart. This type of chemical bond is called a covalent bond [from Latin *co(n)* = with, *valentia* = force, strength].

Covalent bonds between atoms can lead to the formation of a group of atoms called *molecules* [from Latin *moles* = mass, *molecula* = diminutive of moles]. Water (H_2O), for example, consists of water molecules containing one oxygen atom and two hydrogen atoms each. The individual atoms in such a molecule are held together by covalent bonds.

Overview Graphic as a Roadmap for Learning about Chemical Bonds

In the following, an overview table is presented to students (see Table 17). This overview is revisited every time a new type of bond is introduced and discussed in more detail. This overview is thought to work as a kind of roadmap for students to see where the newly acquired knowledge should be implemented into their mental representation of the concept of chemical bonds. Furthermore, it is expected to further foster students' awareness of the existence of three types of bonds and their ability to distinguish between those. Students are given a simplified version of Table 17, which only contains the filed that are colored. The fields with white backgrounds are only filled out later after having discussed the intermolecular forces while talking about larger molecules and diamond-like structures. This approach should dampen students' cognitive load. Students are then prompted to train what they have learned by a task that makes use of interleaved sequencing of different types of bonds.

Table 17: *Overview of the Three Types of Chemical Bonds.*

Type of Bond	**Ionic bond**	**Metallic bond**	**Covalent bond**		
Type of elements	**Metal and non-metal**	**Metals among themselves**	**Non-metals among themselves**		
Attraction between	**Anions + cations**	**Atomic cores + electron gas**	**Atomic cores + electrons**		
Types of particles or structures	**Large ensemble of ions,** forming an **ionic lattice**	**Large ensemble of atoms**, forming a **metallic lattice**	**Small molecule**	**Huge molecule**	**Large ensemble of atoms,** forming an **atomic lattice**
Substance class	**Ionic substances (salts)**	**Metallic substances (metals)**	**Low molecular weight substances**	**High molecular weight substances**	**Diamond-like materials**
Figures					

Note. The table is revisited many times and used as a roadmap. The fields with a white background are not shown to students at the beginning. Sources of figures used in this table: sodium chloride (Benjah-bmm27, 2007), metallic bond (ARTE, 2007), high-molecular-weight substance (Fvasconcellos, 2009), diamond illustration (Cmglee, 2013)

4.5 Fostering Students’ Awareness of the Differences between the Three Types of Chemical Bonds

How can we efficiently bring across the fact that *(2) “there are major differences between the bonding types”*? One approach to make the differences more salient to students is comparing and contrasting activities: Therefore, this teaching unit incorporates many comparing and contrasting activities that foster analogical learning. Such activities have proven to be successful catalysts to foster students’ awareness of the abstract principle behind a concept and foster the visibility of the differences when similar concepts are compared to each other (Alfieri et al., 2013; Gentner, 2010; Ziegler et al., 2020). The method of comparing and contrasting is incorporated into the teaching unit in different ways:

1. Making use of comparing and contrasting activities’ positive effect on difference-detection
2. Incorporation of a reoccurring conductivity experiment with comparing and contrasting character
3. Back referencing to previously discussed types of bonds whenever possible

Making Use of Comparing and Contrasting Activities’ Positive Effect on Difference-Detection

As has been discussed in more detail in chapter 3 of this thesis comparing and contrasting activities bare a great potential for analogical learning in general. Previous work in education research conducted in classrooms in the context of learning about mathematical concepts has shown great potential (Rittle-Johnson & Star, 2007, 2011; Star & Rittle-Johnson, 2009; Ziegler et al., 2018, 2020; Ziegler & Stern, 2014, 2016). There is so far no indication why the method should not work in principle for educational purposes of chemical concepts like chemical bonds. During the process of comparing and contrasting similar concepts, the learning processes of *abstraction* and *difference-detection* are most pronounced in students (Gentner, 2010). It is important to state that the positive effect of comparing and contrasting goes beyond simply knowing the differences when two or more similar concepts are compared. While comparing the ionic bond to the metallic bond, for example, students will not only foster their knowledge about the differences. While students compare those two bonding types students will also automatically think more about the model of the ionic and the metallic bond itself and see the outlines of the concept of the different bonding situations more clearly since they see what is characteristic of the specific bonding type. Therefore we incorporated as many comparing and constricting activities as possible. In total 27 activities make use of *comparing and contrasting* in this teaching unit (45 learning activities in total). Table 18 gives an overview of the methods that find an application in this teaching unit. The method of *comparing and contrasting* is by far *the* most frequently used. Methods that contain comparing and/or contrasting activities, e.g.

inventing with contrasting cases (ICC) or holistic mental model confrontation (HMMC) are counted for both categories. Methods that contain elements of analogical learning are indicated as such in Table 18. A more detailed version of this table can be found in appendix 3.

Table 18: Number of Learning Activities Assigned to a Method of Instruction

Method used in Teaching Unit	*Number of Learning Activities*	*example*
compare and contrast*	27	Figure 31, p. 89
compare*	9	Figure 23, p. 77
inventing with contrasting cases (ICC)*	10	Figure 26, p. 80
experiment containing comparing and contrasting characteristics*	7	Next section, p. 90 onwards
holistic mental model confrontation (HMMC)*	1	Figure 68, p. 136
interleaved practice*	3	Figure 38, p. 100
making use of analogy*	3	Chapter 4.4, p. 82, onwards
pre-structured concept map	2	Figure 41, p. 104
self-explanations	6	Figure 70, p. 138
cognitively activating introduction	4	Polyatomic ions, p. 98
productive failure	1	Figure 53, p. 119
common practice	5	See appendix 3, Teaching Materials, chapter 5.7
training of procedural knowledge	4	See appendix 3, Teaching Materials, chapter 2.2

Note. * Methods indicated with an asterisk make use of analogical learning (i.e. either comparing and contrasting or another analogical learning process). Since comparing and/or comparing are an integral part of some other methods (e.g. ICC or HMMC) some activities were counted for both categories.

Note: The teaching materials are given the name comparing and contrasting teaching materials for the reason that this method finds its way into most of the learning activities (27 of 45). However, it must be stated that not every content is best taught using the method of comparing and contrasting. The teaching materials were designed such that they would take up the same amount of time as conventional instruction. Examples of the instructional methods used in the teaching materials are given in Table 18, right column.

There are various comparing and contrasting activities in the teaching unit. In the following, an exemplary task is shown (Figure 31).

Exercise 1: Hugo believes that metallic substances are salts, which are composed only of positive ions (cations).

a) Why would such a compound be completely unstable?

A compound made of cations only would be completely unstable, because cations repel each other.

b) List the similarities and differences between salts and metallic substances to show him that it makes sense to distinguish salts from metals.

Similarities

- Regular arrangement
- Many atoms/ions form a lattice
- Often present as a solid at room temperature

Differences	**Ionic compounds (salts)**	**Metallic compounds (metals)**
Type of elements contained (metals M, non-metals NM)	NM/M	M
Built from…	Anions and cations	Atomic core + electron gas
Localization/mobility of the valence electrons	The valence electrons are localized at the anions	Free to move in the solid
Particles are held together because of…	Attraction between cations and anions	Attraction between the valence electrons of the electron gas and the atomic cores
Conduct electrical current	If liquid	Also as solid
Brittleness/Malleability	brittle	Malleable/high ductility

Figure 31: Exemplary comparing and contrasting task. Solutions are indicated in green.

Incorporation of a Reoccurring Conductivity Experiment with Comparing and Contrasting Character

Experiments are an important method in every chemistry educator's toolbox: Showing a chemical or physical phenomenon to students can help students to understand a certain concept or an interesting question that needs to be addressed. Chemical experiments can also be used to foster students' awareness of the limitation of their knowledge when students see a phenomenon they cannot explain with their known concepts. This can then be used to foster students' motivation to learn about a new concept. In such a setup an experiment can be used in the sense of a productive failure ((Kapur & Bielaczyc, 2012). Those aspects are used in a developed conductivity experiment that is reoccurring multiple times during the curriculum about chemical bonds. The experiment is used as the introduction for the in-depth introduction of each bonding type (red arrows in Figure 32). The experiment is set up in three stages with increasing complexity:

- Part I: Introduction of the concept of electrical conductivity and the nature of the ionic bond
- Part II: Introduction of the metallic bond and the difference from the ionic bonding situation
- Part III: Introduction of the covalent bond and the differences between ionic and metallic bonds

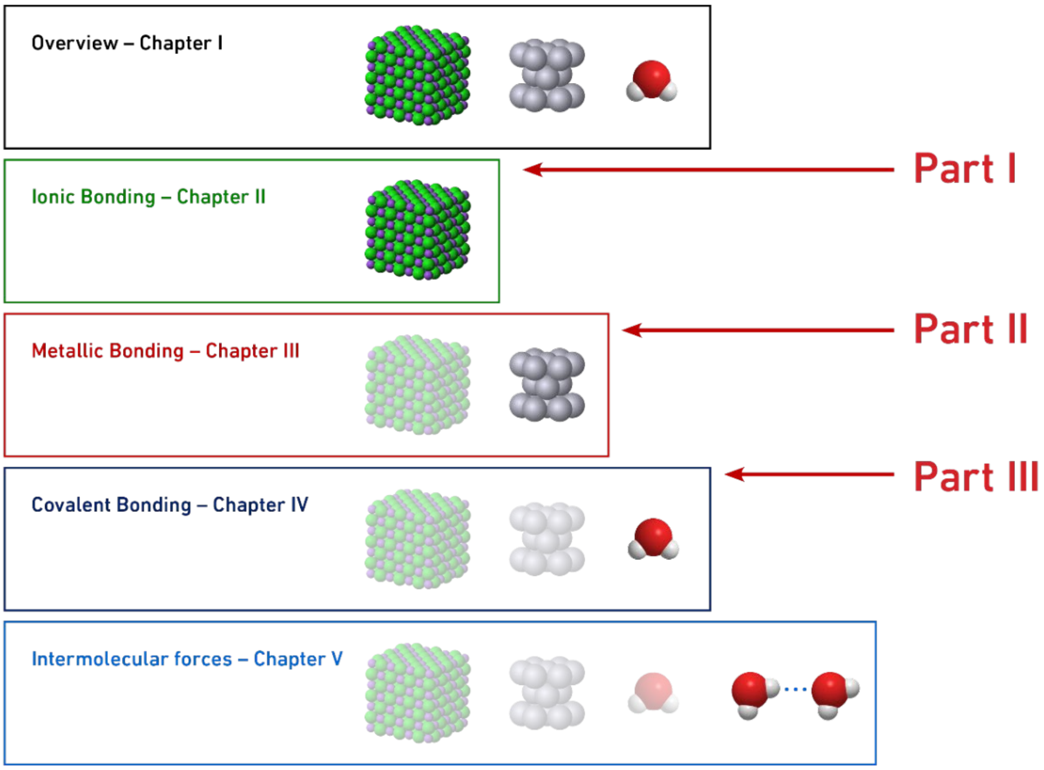


Figure 32: Overview illustration for the teaching unit with localization of conductivity experiment (red arrows). The experiment is increasing in complexity and setup in three stages (Part I to III).

Part I: Introduction of the Concept of Electrical Conductivity and the Ionic Bonding Situation

In the Swiss school system, the concepts of electricity and conductivity are briefly discussed in physics classes at the secondary level I (grades 6 to 9). Nevertheless, instruction in more detail is only discussed in physics classes to come at the Gymnasium. Therefore the concept of conductivity needs to be introduced to students. To activate students' thought processes I ask students whether water possesses electrical conductivity or not. Also without in-detail knowledge students possess experiences from daily life and they know that it is not a good idea to take a bath with the hair drier plugged in. Therefore, it comes as a surprise to most students when it can be shown that distilled and pure water does not possess great conductivity as is observed via a conductivity meter (Figure 33). At this point, it makes sense to talk about what the difference is between what chemists define as the substance water (distilled, pure H_2O) and what is commonly known as tap water. In the follow-up experiment, it can be shown that tap water does in fact conduct electricity and the general warnings on electrical devices have their right to exist. However, the question of what the difference is between tap water and pure water remains. Tap water contains ions in considerable amounts from sedimentation and gas up-take processes, while pure water does not or much less so - neglecting the intrinsic dissociation and the small concentrations of OH^- and H_3O^+ of water for the moment.

This sets the stage to discuss the conditions that must be met for electrical conductivity:

1. The substance must contain electrically charged particles.
2. The electrically charged particles must be able to move freely.

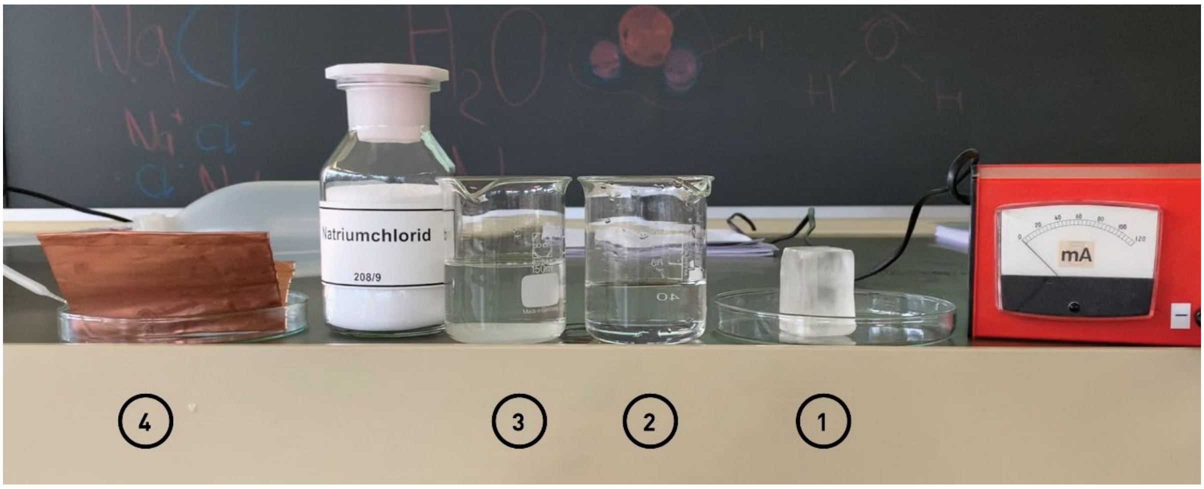


Figure 33: Conductivity experiment with increasingly complex setup. The electrical conductivity of a solid sodium chloride crystal (1), distilled water (2), water with dissolved sodium chloride (3), and a metallic substance (4) is investigated using a conductivity meter (red).

With this in mind, the experiment is expanded to find out about the electrical conductivity of a solid sodium chloride crystal (number 1 in Figure 33) and sodium chloride dissolved in water (number 3 in Figure 33). Students are then prompted to make logical inferences based on the conditions that must be met for conductivity to be observed (see Worksheet II/1, appendix 3). Students generally recognize that particles in a liquid substance are free to move whereas this is not the case for solids using the known particle theory. In conclusion, students will fill out Table 19 and should conclude that a solid sodium crystal does contain ions, but they are not free to move and hence explaining the lack of electrical conductivity. With this students have already encountered the most important facts about the nature of the ionic bond and ionic substances in general.

Table 19: Table from Worksheet II/1 to summarize the observed phenomena and the conditions for electrical conductivity.

Substance	*Tap water*	*Distilled water*	*Sodium Chloride (table salt)*	*Sodium chloride dissolved in water*
Electrical conductivity	yes	no	no	yes
Free moving particles	yes	yes	no	yes

Part II: Introduction of the Metallic Bond and its Difference from the Ionic Bonding Situation

The experiment is revisited and expanded after students have discussed the nature of the ionic bond in more detail. At the beginning of chapter III, covering the in-depth discussion of the metallic bond and metals, the conductivity experiment is extended with the conductivity measurement of a solid metallic substance (aluminum foil). Additionally, the melting points of the substances are given. Students are again prompted to think about the implication of the fact that aluminum foil exhibits strong electrical conductivity in its solid physical state. This seeming contradiction should activate students' prior knowledge and make them aware that metals are fundamentally different from ionic compounds. At that point, students are shown the overview roadmap (see Table 17, page 86) and made aware that it is not surprising that we observe different properties of electrical conductivity since we are looking at substances with a new type of chemical bonding: metallic bonding.

The experiment is developed further by discussing the different melting points of the investigated substances. This highlights the fact that cohesion forces must be present in metals since most metals are in a solid state at room temperature. The observations are summarized in Table 20.

Table 20: Table for the summary of the results from the conductivity experiment part II. A metal (aluminum foil) is added as well as the melting points of the substances (marked in red).

Substance	*Pure water*	*Sodium chloride (table salt)*	*Sodium chloride dissolved in water*	*Aluminum foil*
Electrical conductivity	no	no	yes	yes
Free moving entities/particles (yes/no)	yes	no	yes	yes
Melting point	0 °C	~ 800 °C	-	660 °C

The observations of the experiment motivate the deduction of three inferences:

1. Metals also conduct electricity in the solid state, whereas salts do not.
2. There must be freely moving charged particles in solid metallic substances.
3. High melting point: There must be a reason for the metallic atoms to hold together.

Those inferences lead to the following questions:

1. Which charged particles are free to move in solid metallic materials?
2. How do the atoms in solid metals exist?
3. How do the metallic atoms hold together?

Those questions are the starting point to discuss the nature of the metallic bond and its differences from the previously discussed ionic bonding situation. The simple model of the electron see is introduced at this point (for details see chapter III of the teaching unit, appendix 3).

Part III: Introduction of the Covalent Bond and the Differences between Ionic and Metallic Bonds

Revisiting the conductivity experiment at the start of chapter four helps students prepare for the in-depth discussion of the covalent bond. Students are made aware of a result they have encountered all along without paying too much attention: Water does not conduct electricity even though the contained particles are free moving – apparent due to the liquid state. To complement the experiment solid ice is introduced and tested for its conductivity (see Table 21).

Table 21: Table for the Summary of the Results from the Conductivity Experiment Part III.

Substance	*Sodium chloride (table salt)*	*Aluminum foil*	*Ice (solid)*	*Pure water (liquid)*
Electrical conductivity	no	yes	no	no
Free moving entities/particles (yes/no)	no	yes	no	yes

Revisiting this observation and focusing on the substance water in the solid and liquid state three inferences are made:

1. Pure water does not conduct electricity, even in its liquid state.
2. Water must contain electrically neutral particles (i.e. no ions).
3. In its solid state (ice), water has no free-moving valence electrons (as is the case for metals).

The observations of the simple conductivity experiment help students see that water contains no ions, i.e. cannot be an ionic substance or contain ionic bonds. Additionally, the observed conductivity behavior does not match the properties of a substance with metallic bonding. Again, at that point the overview roadmap (see Table 17, p. 86) is consulted: Water is comprised of water molecules with the molecular formula H_2O, hence only non-metallic elements are present in the substance. Following what has been learned before students will see that this would typically lead to covalent bonds being present in a substance with the formation of small molecules. The experiment should raise awareness for their limited understanding of the covalent bonding situation and hence foster their motivation to learn about the new concept.

As a next step, students are introduced to another substance composed of non-metals: Hydrogen gas. It might come as a surprise for students to see that the substance composed of the element hydrogen is in the gaseous state. Students are then prompted to think about the reasons behind the relatively low melting points of hydrogen gas (H_2) and water (H_2O) in comparison to sodium chloride ($NaCl$) and aluminum foil (Al) (see Worksheet IV/1, appendix 3).

Table 22: Comparison of Different Substances' Melting Points.

Substance	*Sodium chloride*	*Aluminum foil*	*Pure water*	*Hydrogen*
Physical state at room temperature	solid	solid	liquid	gaseous
Melting point	~ 800 °C	660 °C	0 °C	-259.2 °C

Note. Substances composed of non-metals (water and hydrogen gas) show lower melting points than sodium chloride and aluminum foil.

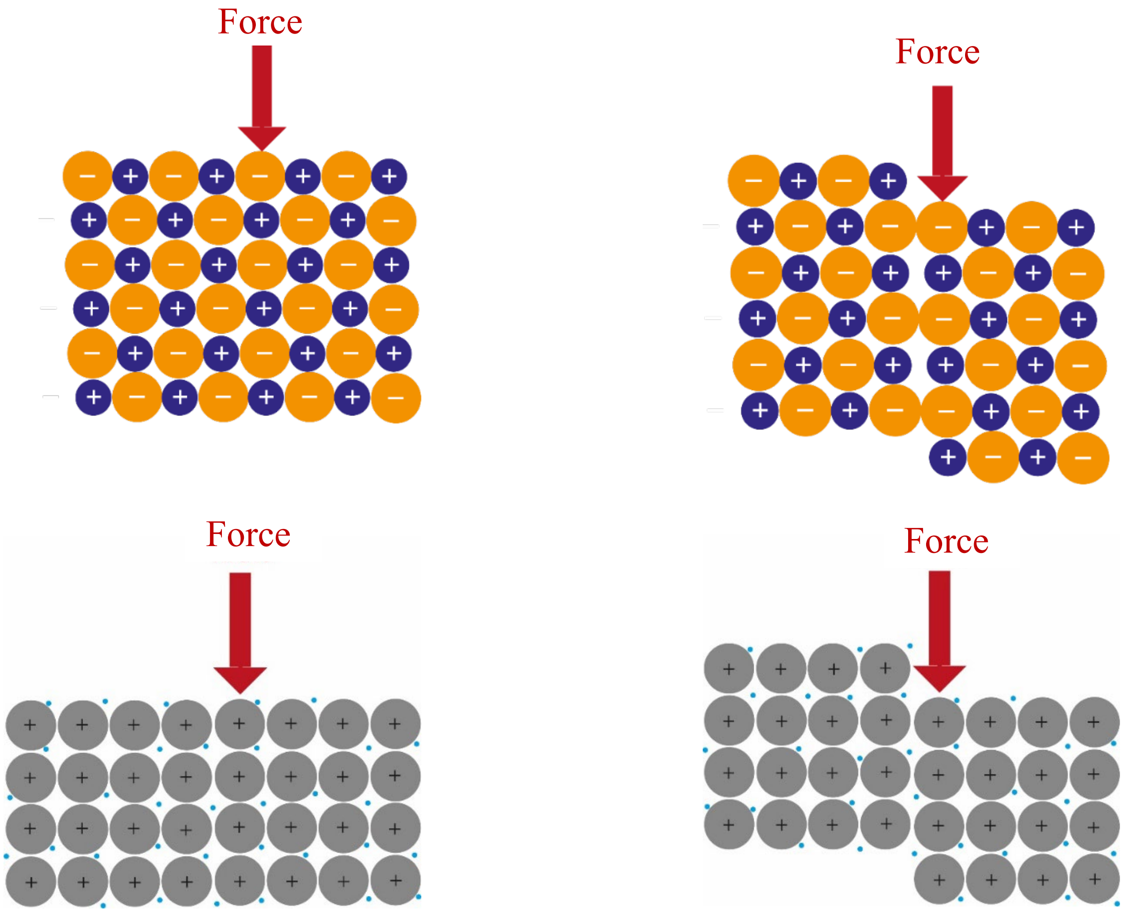
Students are made aware of the fact, that the building of stable subunits, i.e. molecules, is a characteristic specific to molecular substances composed of non-metals and is not observed in metals and salts. It is important to acknowledge that the melting points of substances containing molecules are in fact low. But at this point, it is most prudent to stress that this does not directly lead to the conclusion that covalent bonds are weak. Instead, it must be stated that the attracting forces between the molecules, i.e. the *intermolecular forces*, are much smaller than the attraction between ions in salts, and those between the atomic cores and the electron gas in metals. The topic of intermolecular forces will be discussed in chapter five of the teaching unit but the statement and differentiation between inter- and intramolecular attracting forces are made at the very beginning of the in-depth discussion of the covalent bond. Results previously discussed in this thesis suggest that students have difficulties distinguishing between inter- and intramolecular forces and their effect on surface properties like boiling and melting points (see p. 41 for more detailed discussion).

Back Referencing to Previously Discussed Types of Bonds Whenever Possible

Typically the sequence of instruction for the different bonding types is strict and interleaving of different bonding types is avoided. We on the other hand promote the implementation of comparing and contrasting activities between the different bonding situations whenever possible. In the following, I will present a few of the possible back-references that can be implemented, when teaching about the different types of chemical bonds.

1. Comparison of the Ductility of Ionic Compounds and Metallic Substances

Instruction time is limited. Therefore, efficient ways how to compare different types of bonds are welcome. In the following example (see Figure 34) students are prompted to compare what happens if ions or atomic cores are shifted. Instead of discussing the reason for the brittleness of sodium chloride, already when talking about salts (chapter two of the teaching unit), the comparison is only made after metallic substances are introduced in chapter three. This will save time since the reason for the brittle character of salts respectively the high ductility of metals can be discussed at the same time. While students compare the different bonding situations and the result of a shift, they automatically compare the different bonding situations and will see the differences between the two bonding models more clearly.



Before the force is applied

After the force is applied

Figure 34: Exemplary comparing task between the ionic and metallic bonding situation. The students will reactivate their prior knowledge about ionic bonds and compare what they have learned so far with the metallic bond. For the complete exercise see worksheet III/1, appendix 3.

2. Discussion of Polyatomic Ions

What types of chemical bonds can be expected in a substance with the chemical formula NH_4Cl? This question is presented in the classroom after students have already learned about all three types of chemical bonds in detail. At this point, students will have acquired the needed procedure and check for the presence of metallic and/or non-metallic elements: All the elements present in NH_4Cl are non-metallic, therefore, we would expect a molecular substance and NH_4Cl molecules. In the following, the substance is shown to the students: NH_4Cl, a solid crystalline substance, looks similar to sodium chloride. Students are then prompted to think of ways how we could further test the hypothesis of an ionic or molecular substance. The property of electrical conductivity can be used at this point. While there is no conductivity in the solid state, there is strong conductivity when the substance is dissolved in water. This will confuse students for a while, but this temporary confusion can be used to refocus the attention to a more complex substance class of ionic compounds containing molecule-ions.

Molecules are generally net neutral, as has been shown by the lack of electrical conductivity of water. Unfortunately, from a didactic point-of-view, the chemical reality is more complex. Some molecules can be classified as Brønsted bases and acids. This means that under certain circumstances a before-neutral molecule can accept an additional proton (H^+) which results in a molecule with a net positive charge (see Figure 35). Such molecule ions are also called polyatomic ions. The subject of acids and bases is an important topic in the chemistry curriculum and is hence discussed in more detail at a later stage. The topic can be introduced on a basic level to understand the nature of polyatomic ions.

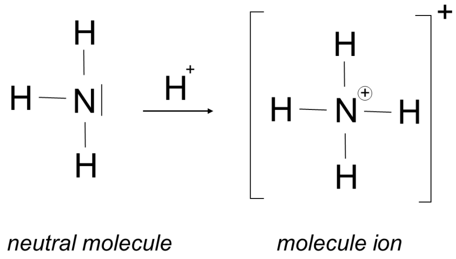


Figure 35: Illustration of the building of a molecule ion. In proton-transfer processes, neutral molecules (e.g. ammonia, NH_3) become positively charged (e.g. ammonium, $(NH_4)^+$). Such molecule ions, also called polyatomic ions can be used as regular building blocks for ionic compounds.

Such molecule ions can be implemented as building blocks of an ionic compound (e.g. NH_4Cl, see Figure 36). Following the idea of didactic simplification, it would be a valid approach to neglect such ionic compounds. Ionic compounds containing polyatomic ions are very common and can hardly be neglected at all. Instead of making a detour around the complicated topic, this teaching unit embraces the welcome possibility to take up the ionic bonding situation and discuss how it is possible to form an ionic compound containing exclusively non-metallic atoms. Students are made aware that there are in fact covalent bonds present in NH_4^+ but the overall nature of the compound is of ionic nature. The positively charged ammonium cation and the negatively charged chloride anion hold together via electrostatic interaction as has been previously observed for ionic compounds with common ions. The fact that this substance is a solid crystalline structure at room temperature and only conducts electricity upon dissolution in water supports this classification.

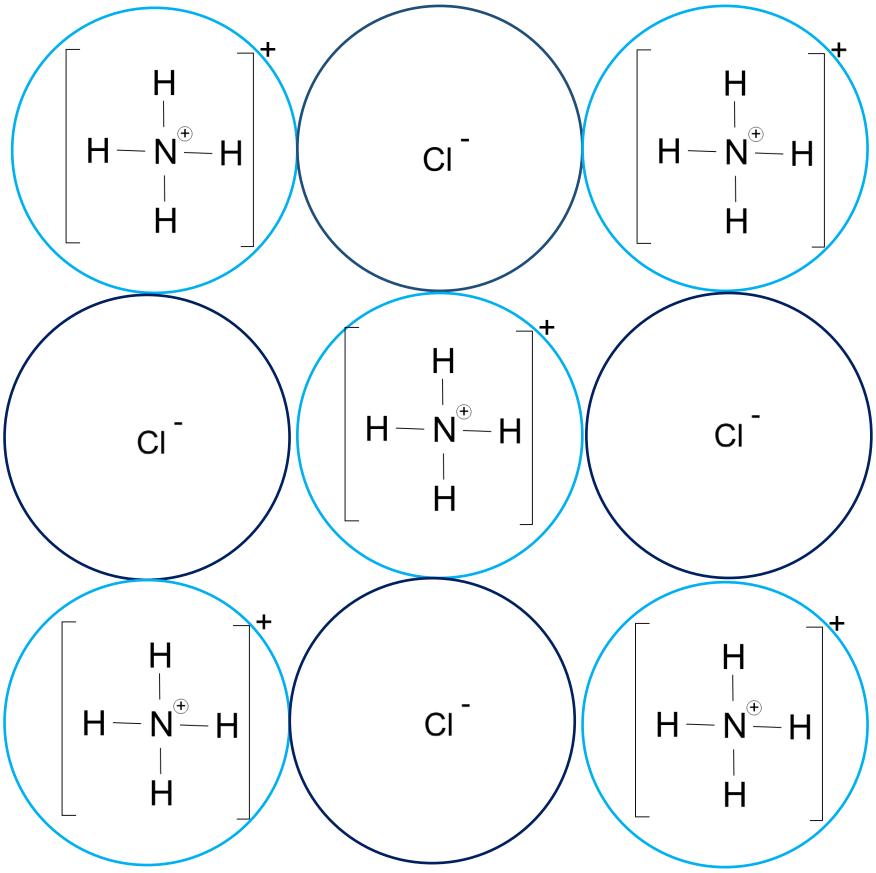


Figure 36: Illustration of ammonium chloride (NH_4Cl) an ionic compound comprised of chloride anions and a positively charged molecule cation (NH_4^+).

Other molecular substances can be classified as Brønsted acids. This means that if diluted in water such molecules tend to dissociate a proton (H^+) and thereby acquire a negative net charge. The list of common molecule anions is longer but less problematic for students (see Table 23 for some examples). Since they often occur in combination with cations that are of metallic elemental nature and are hence easier to recognize as such upon being presented in a chemical formula.

Table 23: List of Common Polyatomic Anions

Hydroxide	$(OH)^-$
Nitrate	$(NO_3)^-$
Bicarbonate	$(HCO_3)^-$
Carbonate	$(CO_3)^{2-}$
Sulfate	$(SO_4)^{2-}$
Phosphate	$(PO_4)^{3-}$

Chalk (calcium carbonate, $CaCO_3$), a substance also known to students, is a typical representative of such an ionic compound. Students are shown the reaction of an acid with $CaCO_3$ and see that the substance foams and is decomposing in the process. The molecule anions can be forced to take up two protons and hence lose their ability to stabilize the ionic compound. The observed gas is carbon dioxide (CO_2) which is formed via the decomposition of H_2CO_3 into H_2O and CO_2.

In conclusion, students are made aware of the fact that the simple heuristic to classify by occurrence of non-metallic and/or metallic elements in a substance holds in almost all cases, but students need to be on the lookout for ammonium (NH_4) in chemical formulas.

3. Interleaving of Ionic Compounds when Drawing Lewis Structures of Molecules

Once students are instructed in how to draw Lewis structures students usually get immersed in the process. Usually, it takes a while to train the typical procedures of how to correctly draw the Lewis structure of simple molecules. Gilbert N. Lewis postulated the easy-to-use chemical language in his article called “The Atom and the Molecule” (Lewis, 1916). Not only is it an elegant way of how to draw simple molecules it is a way of how *to predict* the covalent bonding situation of simple molecules and is therefore still taught nowadays and widely used. It can be said that the Lewis structure way of drawing is the chemists' own language. It is therefore not surprising that students are prompted (or forced with external motivation) to typically spend a fair amount of time learning how molecules are drawn and predicted with the method of drawing Lewis structures. However, this leads to a new problem: Students tend to forget about other types of bonds after they have worked extensively on tasks of how to draw molecules. Sometimes students will also wrongfully transfer the procedures for predicting the structure of molecules onto situations where this is not applicable. A typical mistake would be that metallic atoms are drawn in the Lewis dot formula form. Since usually students are used to combining single valence electron dots to lines to formulate covalent bonds some of them transfer that procedural knowledge to sodium chloride (see Figure 37). Students might get the idea that a sodium chloride molecule exists in such a form and might add a rationale for the prevalence of the misconception of sodium chloride molecules.

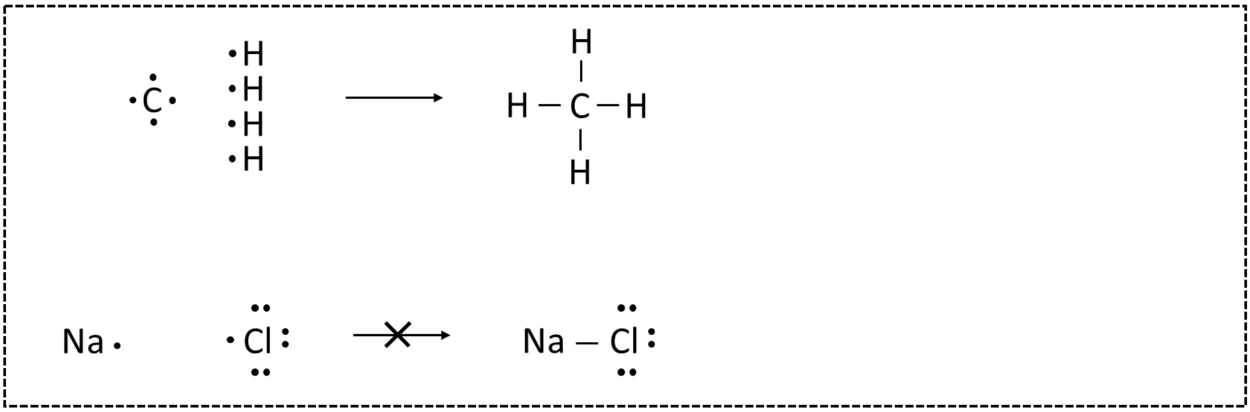


Figure 37: Illustration of the wrongful transfer of procedural knowledge concerning the formulation of Lewis structures.

To prevent this undesirable transfer of procedural knowledge, a task where this transfer should not be made is casually implemented in exercises where students are supposed to draw Lewis structures of molecules (see

Figure 38). After students have finished their exercises the solution is discussed. Typically, many students would fall into the laid-out "traps". The important point is to make, that even though they are currently working on a new and sometimes challenging procedure to learn they should not forget about the overall picture and the general procedure of how to identify the bonding type before blindly following common procedure.

Question 1: Find the Lewis structure of the following substances. Which compound is formed from…

a) One atom of carbon (C) and four atoms of fluorine (F)

b) Two atoms of fluorine (F) and one atom of oxygen (O)

c) One atom of hydrogen (H) and one atom of chlorine (Cl)

d) One atom of potassium (K) and one atom of chlorine (Cl)

e) One atom of nitrogen (N) and chlorine atoms

f) An atom of magnesium (Mg) and an oxygen atom (O)

Figure 38: Example from the teaching unit of how interleaving of ionic compounds (marked in red) can help build up resistance against the undesirable transfer of procedural knowledge.

Students' flexibility in changing between different bonding types is further fostered: In between tasks to find the correct Lewis structures of molecules, they are given self-explanation tasks with comparing character. Some chemical formulas are very similar on the surface level: HCl and KCl for example share great similarities. Therefore, we interleaved a self-explanation task where students have to compare similar chemical formulas and elaborate on the difference between the discussed substances. An example is given in Figure 39.

Question 2: Hugo claims that HCl and KCl are structurally very similar and that one can simply replace the H atom in the HCl molecule with a K atom. Explain to him how the two substances differ from each other.

Figure 39: Self-explanation task to foster students' ability to distinguish between substances with similar chemical formulas but different bonding situations.

4. Revisiting the Comparison of a Diamond, Ice, and Sodium Chloride Crystal

When all the bonding types (chapters I to IV) and an introduction to intermolecular forces (chapter V) have been taught, the introduction task of comparing ice, sodium chloride, and diamond (see Figure 23) is discussed again. When asked about the reasons behind the differences in the melting temperatures of those substances the first time, students did not have the appropriate concepts at hand to explain the phenomena. In the sense of a circular curriculum, students will be directed to think again about the before-handed question of how to explain those differences and similarities.

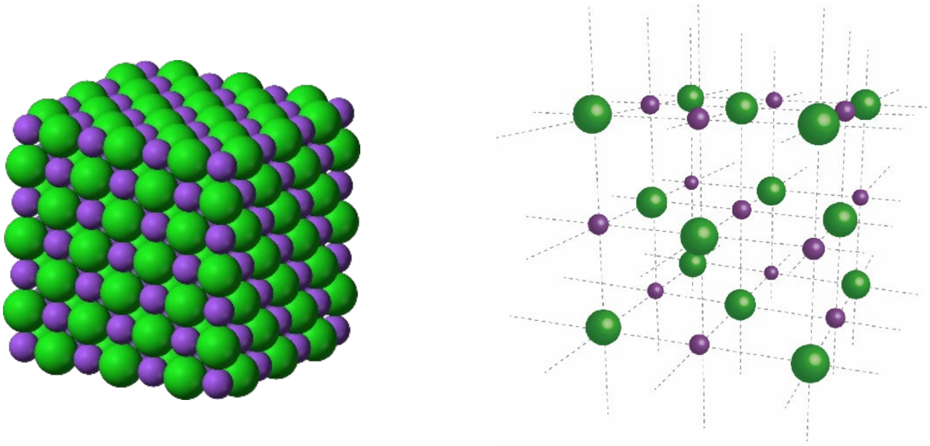
Students are prompted to compare the crystalline structure of sodium chloride and water in a solid state (see Figure 40). Thereby revisiting their representation of the concepts of ionic bonding, respectively the characteristics of ionic compounds as well as the concept of covalent bonding, the formation of molecules, and the intermolecular interaction between water molecules. Students are made aware of the differences between those two substances with follow-up questions.

In conclusion, students should be able to fully explain the difference in melting points of water and sodium chloride: To change the physical state of water from solid to liquid intermolecular forces need to be weakened, while in the case of sodium chloride, the ionic bonding situation between ions is disrupted. Since intermolecular forces are weaker by different orders of magnitude, the lower melting point of water is explainable.

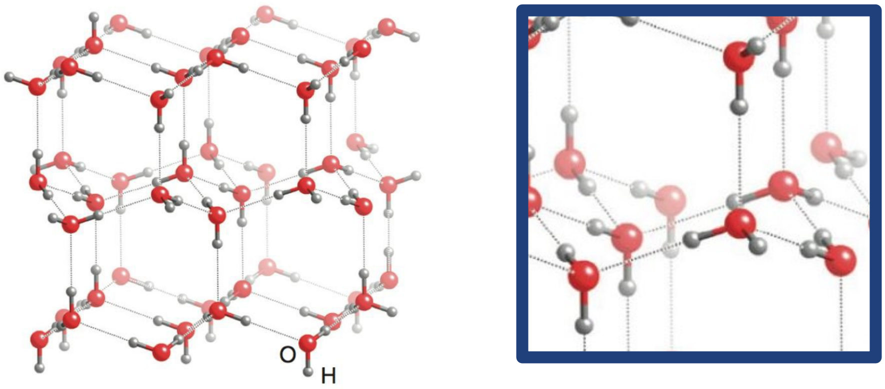
In the following students are asked to explain why water (H_2O) and diamond (C) have such different melting points. Since both substances are exclusively comprised of non-metallic elements, we would expect covalent bonds to be present in both substances. Yet, the difference in the melting points between water (0 °C) and diamond (approximately 4000 °C) is vast. Diamond is comprised of exclusively one element – carbon a non-metal. Therefore, we would expect a covalent bonding situation and molecules. How can we explain the high melting point even though the intermolecular forces are usually relatively weak? The answer to this question is quite simple: There are no intermolecular forces present in a diamond. All the carbon atoms are bound covalently with each other. Every carbon atom is covalently bound to four other carbon atoms. One could say that a diamond is one single huge molecule. To observe the liquid and finally the gaseous state of a diamond (single carbon atoms) we thus have to break up covalent bonds between the carbon atoms. Of course, these processes only occur at very high temperatures and therefore explain the high melting and boiling temperatures of diamonds.

Students are then motivated to look at their prior guesses of how to explain the differences and hopefully see how much they have accomplished and how far they have come since starting to learn about chemical bonds.

Question 1: Compare sodium chloride (NaCl) in the form of a salt crystal with an ice cube (H_2O)



To get a better look inside the salt, the sodium cations (purple) and chloride anions (green) were drawn slightly apart.



a) Circle two water molecules in the blue-framed figure.

b) How are the atoms present in the two compounds?

c) How are the particles in H_2O held together?

d) How do the particles in NaCl stick together?

e) Draw the intermolecular forces for the substances. What are they called?

f) How many bonding partners do the atoms in bold have? Na**Cl** / H_2**O**

g) Draw water at 100 °C.

Figure 40: The crystalline structure of sodium chloride (top left; Benjah-bmm27, 2007) is compared with crystalline water (Nick Greeves, n.d.). Follow-up prompts are given to make students elaborate on the differences between the two substances with similar surface characteristics.

5. The Use of Pre-Structured Concept Maps

The different bonding types share some similarities but also differ in some aspects. After students have studied the three bonding types in detail (chapters I – IV in the teaching unit) students are asked to fill out the pre-structured concept maps of the three bonding types. To make the differences more salient the three bonding types are represented on one sheet and condensed to the most important facts (see Figure 41). This task will activate students' prior knowledge of all three bonding types and potentially foster awareness of the existence and differences between the three bonding types. Additionally, students' ability to deduce which bonding type is present in a substance is once more discussed before going into the topic of intermolecular forces.

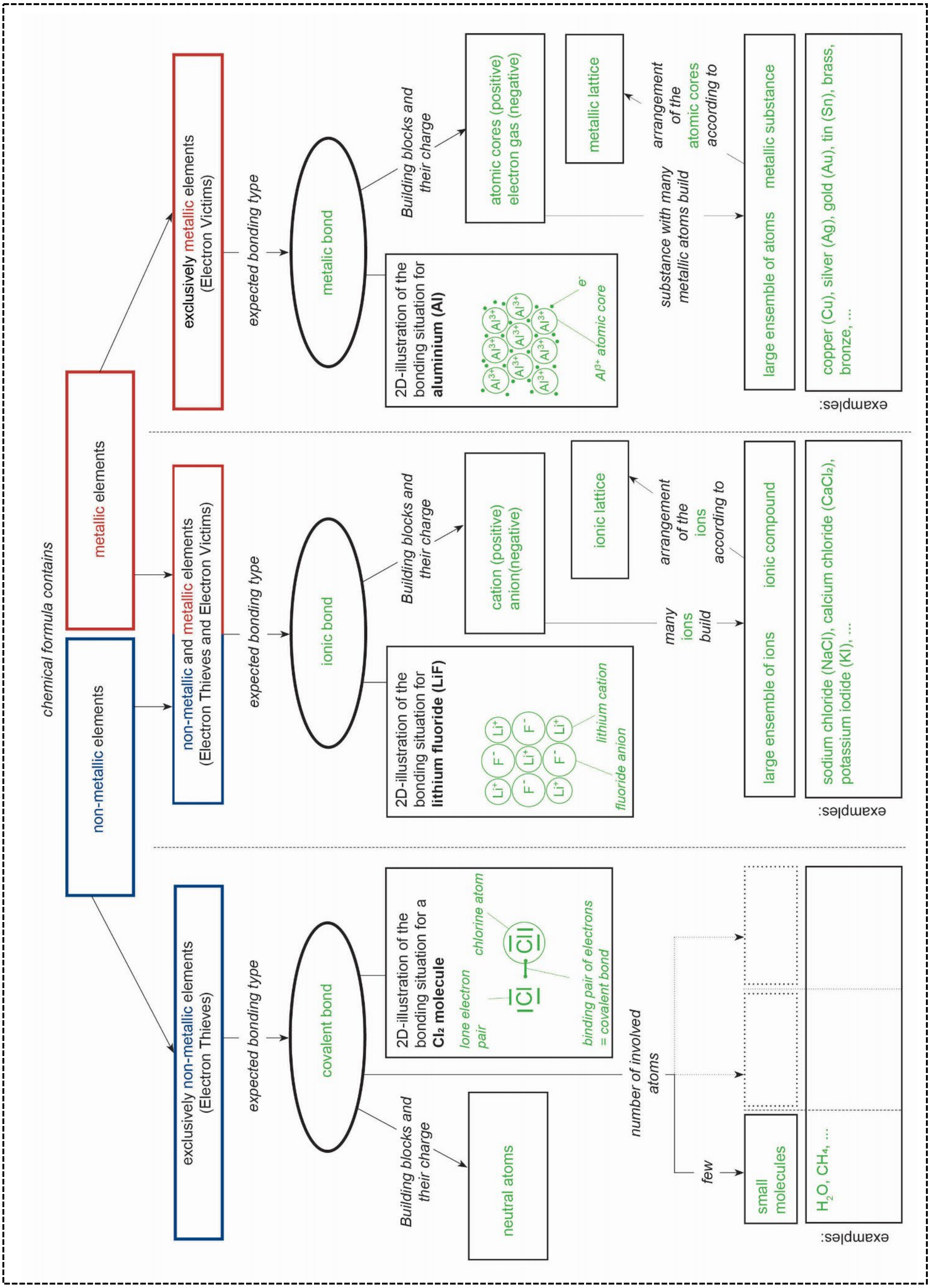


Figure 41: Pre-structured concept map of the three bonding types. Solutions are indicated in green. A similar concept map has been published previously in German in a book chapter the author contributed to (Barth et al., 2022). Reprinted with editor's permission.

4.6 Fostering Students' Understanding of the Cohesion of Atoms and Ions to Form Ensembles

As stated in the introduction, it is my strong belief that chemistry novices can in fact be taught level-appropriate concepts that explain the fundamental behavior of the smallest particles. This means, that *(3) "the strength and the reason behind the attraction of atoms and ions to form ensembles (metals, ionic compounds, and molecules) can be rationalized."*

I hypothesize that one reason for the observed difficulties in understanding is, that students do not have a profound understanding of why the small particles, i.e. atoms, and ions, hold together. Therefore, four ideas are implemented into the teaching unit to foster students' conceptual understanding:

1. Use of Coulomb's law to explain cohesion forces
2. Presentation of a level-appropriate model for each bonding type
3. Giving students a sense of the quantum mechanics theory
4. Explicit declaration of heuristics with further rationalization

Use of Coulomb's Law to Explain Cohesion Forces

Coulomb's law is as simple as useful: There are positive and negative charges. Particles with opposite charges attract each other while particles with the same charge exhibit repellant forces.

The force F_c exhibited by two charges (Q_1 and Q_2) in distance r to each other can be described as the following:

$$F_c = \frac{1}{4 \cdot \pi \cdot \varepsilon_0} \cdot \frac{Q_1 \cdot Q_2}{r^2}$$

The first fraction containing the electric constant ε_0 consists of constant values therefore the equation can be simplified into a qualitative form:

$$F_c \sim \frac{Q_1 \cdot Q_2}{r^2}$$

For chemistry education purposes it is often sufficient to know how the Coulomb force F_c is reacting to variable parameters (Q and r). Qualitatively students should have a sound understanding of the following aspects:

1. Higher charges Q lead to higher Coulomb forces F_c
2. Increasing the distance r between the charges will reduce Coulomb forces F_c in the square

This understanding lays out the foundation for almost all explanations for the phenomena encountered during the curriculum on chemical bonds. It explains central relations, like the attraction of two neutral atoms (see chapter 4.4) or the attraction of electrons and atomic nuclei. It is also the basis for the level-appropriate explanations of bonding types (see p. 106 and following). The attraction of ions of opposite charge, the arrangement of ions in a symmetric lattice, or why ions are often present with full (or empty) shells can be explained. The spatial arrangement of molecules (e.g. tetrahedral arrangement) with the valence shell repulsion model (VSEPR) is also based on the idea of repulsion forces between electron pairs.

Having incorporated the fundamentals of the Coulomb law, teachers can now use the students' ability to make inferences for other central concepts. One of the most central concepts is the understanding of electronegativity: Values of electronegativity can be further rationalized using Coulomb's law. Instead of just giving students the values students can be prompted to find the reasons behind differing values themselves (see p. 78).

Presentation of a Level-Appropriate Model for each Bonding Type

As described in the introduction (see chapter 1), it is not a realistic option to aim for the quantum mechanical model as an introductory model for students to understand chemical bonds. But what are level-appropriate models for students to understand the nature of the different chemical bonds? In the following the models chosen for this teaching unit as well as their limitations and simplifications are briefly described:

Ionic Bonding

To understand the attraction of ions in an ionic compound a sound understanding of Coulomb's law is sufficient. The attraction of positively charged cations and negatively charged anions are held together via the attracting forces. Considering the attraction of ions with the same charge as well as the repulsion of ions with the opposite charges, the arrangement in large ensembles of ions is explicable as well as the arrangement according to a symmetric ionic lattice structure (see p. for how to introduce students to the arrangement of ions). The introduced model is in large part similar to the expert model taught at university. The only simplification is the emittance of the fact that ions can still deform their electron density. The electron density probability of cations will of course be larger in the proximity of the anions and smaller in the regions near other cations. This arrangement further stabilizes an ionic compound and can be seen as a partially covalent character of the bonding situation. It must be stated that the additional stabilization is minor depending on the ions of course. It is a minor didactical simplification to omit this fact.

Metallic Bonding

The stabilization of metallic substances stems from the building of large combined orbitals of many metallic atoms. Seen from an expert's view metallic bonding shares similarities with covalent bonding. The difference is the delocalization of electrons, i.e. the number of involved atoms. While the bonding electrons in metals are delocalized over the whole metal, electrons of covalent bonds are much more localized. The band theory needed to explain the combinations of many orbitals is based on quantum mechanics theory and therefore complicated to explain for chemistry novices.

Typically only one to three lessons are invested to teach about metallic substances and the nature of metallic bonds in standard curriculums at Swiss Gymnasiums. Therefore the introduced model must be rather basic. The model chosen for this teaching unit is the model of *uniform electron gas.* It describes metallic substances as being comprised of atomic cores, i.e. the atoms without the valence shell, and the valence electrons being delocalized over the whole substance. Such delocalized electrons can move freely in between the atomic cores and are called “electron gas” due to their uniform distribution in the space between the atomic cores. According to the model of the uniform electron gas, the reason for the metallic atoms to stay together in an ensemble is the following: The attraction of the positively charged atomic cores exhibits attractive forces towards the negatively charged electrons of the electron gas in between the atomic cores. This holds the atomic cores together and leads to the stability of metallic substances on a macroscopic level. A similar model is more known in the English-speaking part of the world: The *electron sea model*, with the only difference being that the freely moving valence electrons are described as a “sea of electrons” rather than an electron gas. Considering the relative simplicity of the model, its potential for explaining typical properties of metallic substances is surprisingly good. Metallic properties like malleability pronounced heat, and electric conductivity can be rationalized using the model. It is even possible to compare certain metallic substances (containing elements from the main groups) and explain the differences in their properties (see Figure 43).

Exercise 1: Explain the different electrical conductivities of the substances listed. A higher value corresponds to a greater electrical conductivity.

	Sodium chloride (NaCl)	**Aluminum (Al)**	**Sodium (Na)**
Electrical conductivity at room temperature	No conductivity	$37 * 10^6$ A / V m	$21 * 10^6$ A / V m

Sodium chloride is an ionic compound that is comprised of ions. At room temperature, these are held together by the strong attractive forces between the anions and the cations, which are arranged symmetrically (ion lattice) and are not free to move. Since freely moving and charged particles must be present for conductivity, NaCl is not a conductor as a solid.

Aluminum has a significantly higher conductivity than sodium. The conductivity of metals depends mainly on their valence electrons, which have a large free mobility. Since sodium has one valence electron and aluminum has three, it is easy to understand why aluminum conducts electricity better than sodium.

Figure 42: Exercise in which the electron gas model can be used to explain the difference in conductivity of two metals (aluminum and sodium)

Covalent Bonding

Atoms can combine and form molecules held together by covalent bonds. Hydrogen atoms (1 proton, 1 electron) build H_2-Molecules while helium atoms (2 protons, 2 electrons) do not. How can we explain such chemical behavior? With quantum mechanics and the linear combination of atomic orbitals (LCAO), a method of how to explain the behavior would in theory exist. However, as an introductory model, this is highly unsuited for chemistry novices. There are online tutorials that base their explanations on the rule of noble gases: e.g. “the two hydrogen atoms share their electrons, acquiring the electronic configuration of helium – a noble gas.” Others argue even go so far as to use the Niels Bohr model to explain why bonds are formed (see Figure 43).

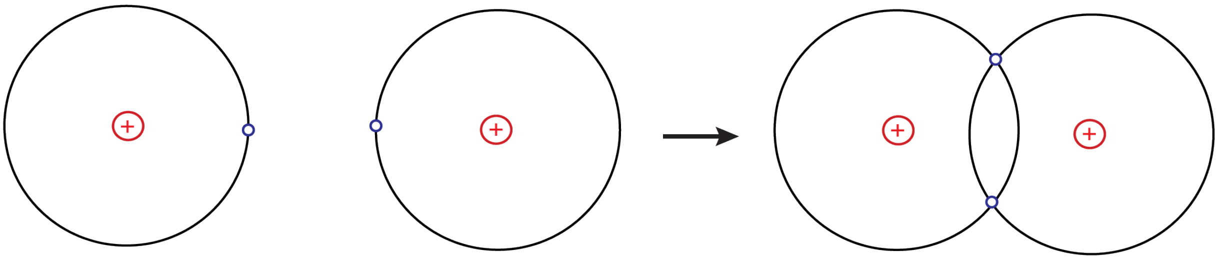


Figure 43: Illustration to explain the formation of H_2-Molecules. Inspired by illustrations found when searching for the formation of H_2-Molecule.

We attempt to aim a little higher than simply reciting heuristics as fundamental explanations. In the next section, I present a method of how to incorporate parts of quantum mechanics to go further than the overlapping of Bohr's shell circles without the necessity of introducing *molecular orbital theory* or the method of the *linear combination of atomic orbitals* (LCAO).

Giving Students a Sense of Quantum Mechanics Theory

I intended to find a way how to give students a sense of quantum mechanical theory without going into details. Quantum mechanical theory is complex and parts of it do not follow the rules of classical physics and electrostatics (e.g. Coulomb's law) which makes it hard to understand since the prior knowledge does not fit the new model. However, we should not forget that parts of it can still be rationalized with what students have already learned (e.g. Coulomb's law with certain restrictions). It is my personal opinion that it is helpful for students to understand that even quantum mechanical theory is not totally arbitrary and follows certain rules and that they can even make educated guesses on the outcome of certain phenomena (electron density, see below). The acceptance of a new model or parts of it is also highly dependent on the fact that they need to understand it at least partially and see the benefits of being able to use it.

At this point students were introduced to atoms with the idea of electrons being located in certain shells, i.e. they are used to the *Bohr shell model*. So the aim is to shift students from the relatively simple model of electron shells towards a more sophisticated model – in this case the *electron cloud model*. The newly introduced model can be seen as a hybrid model to facilitate conceptual change towards the expert model of quantum mechanics which can be introduced in special focus classes (science focus or at university). I am not arguing against the implementation of orbital theory at the Gymnasium level in general. However, I suggest the introduction of this model as a first step for students to make themselves more comfortable with the complex nature of quantum particles. In the following, I present how I intend to give students a sense of the quantum mechanics world.

We introduce electron clouds as simplified atomic orbitals. Therefore students need an understanding of the concept of electron density – i.e. the probability of an electron being present at a certain position. The concept's understanding is facilitated by a prior exercise (see Figure 44).

Question 1: Suppose you are standing at the door of a classroom and you know that the teacher is teaching, but you cannot see into the classroom. Where would you most likely expect to find the teacher? Use a red color to mark areas where the teacher is most likely to be.

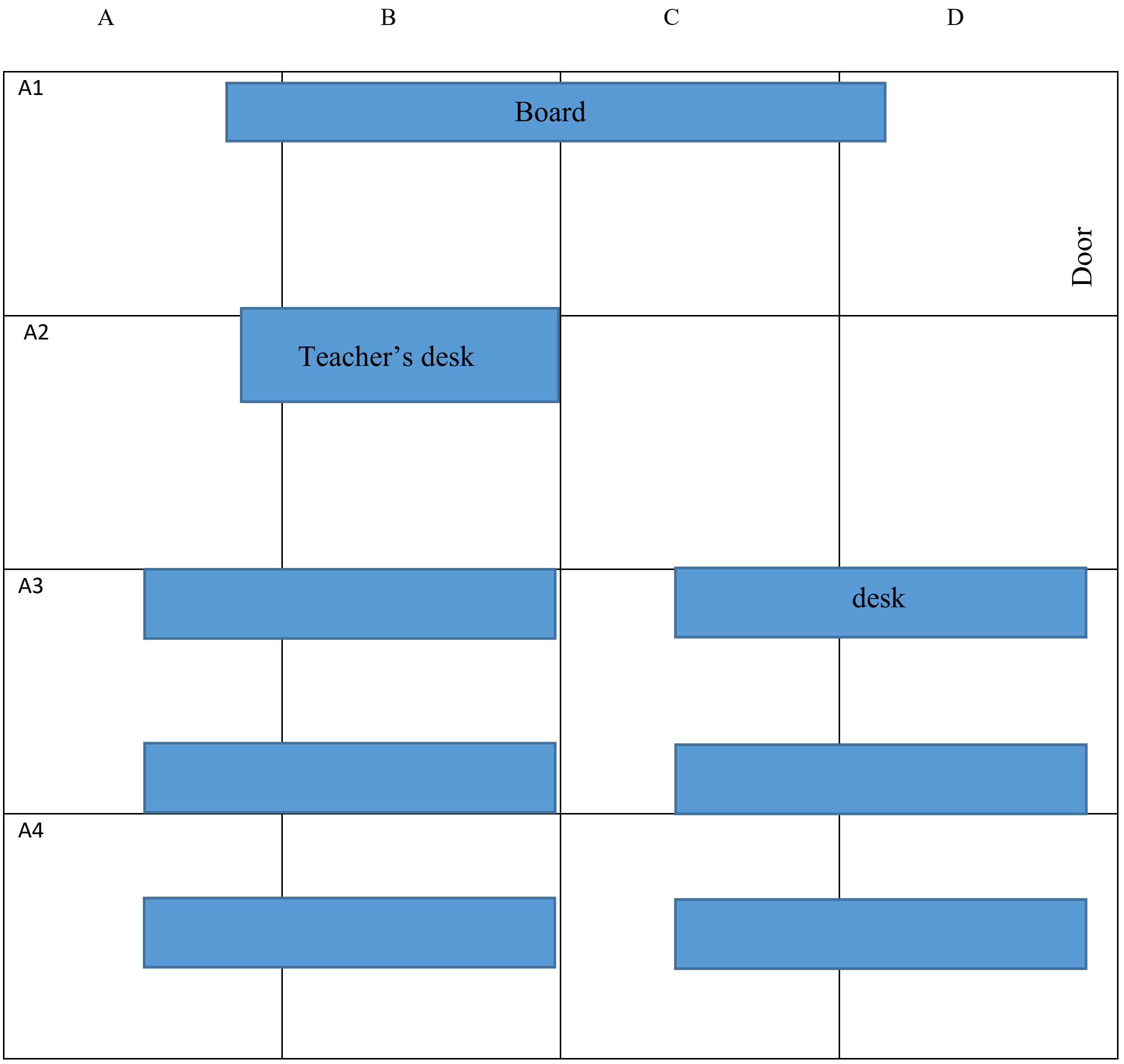


Figure 44: Exercise to facilitate the understanding of the concept of electron density probability

The exercise can be discussed and follow-up questions could be to how the teacher's positioning probability could be changing when different types of lectures are being held (e.g. direct instruction by the teacher, student group work, student presentations). Those follow-up questions prepare students for the fact that the probability to find an electron in a certain position can vary when parameters are shifted, like the addition of another nucleus.

Question 2: Where would you be more likely to find an electron in a hydrogen atom and where less? Which of the four options do you consider as realistic and which not so much? Justify your answers.

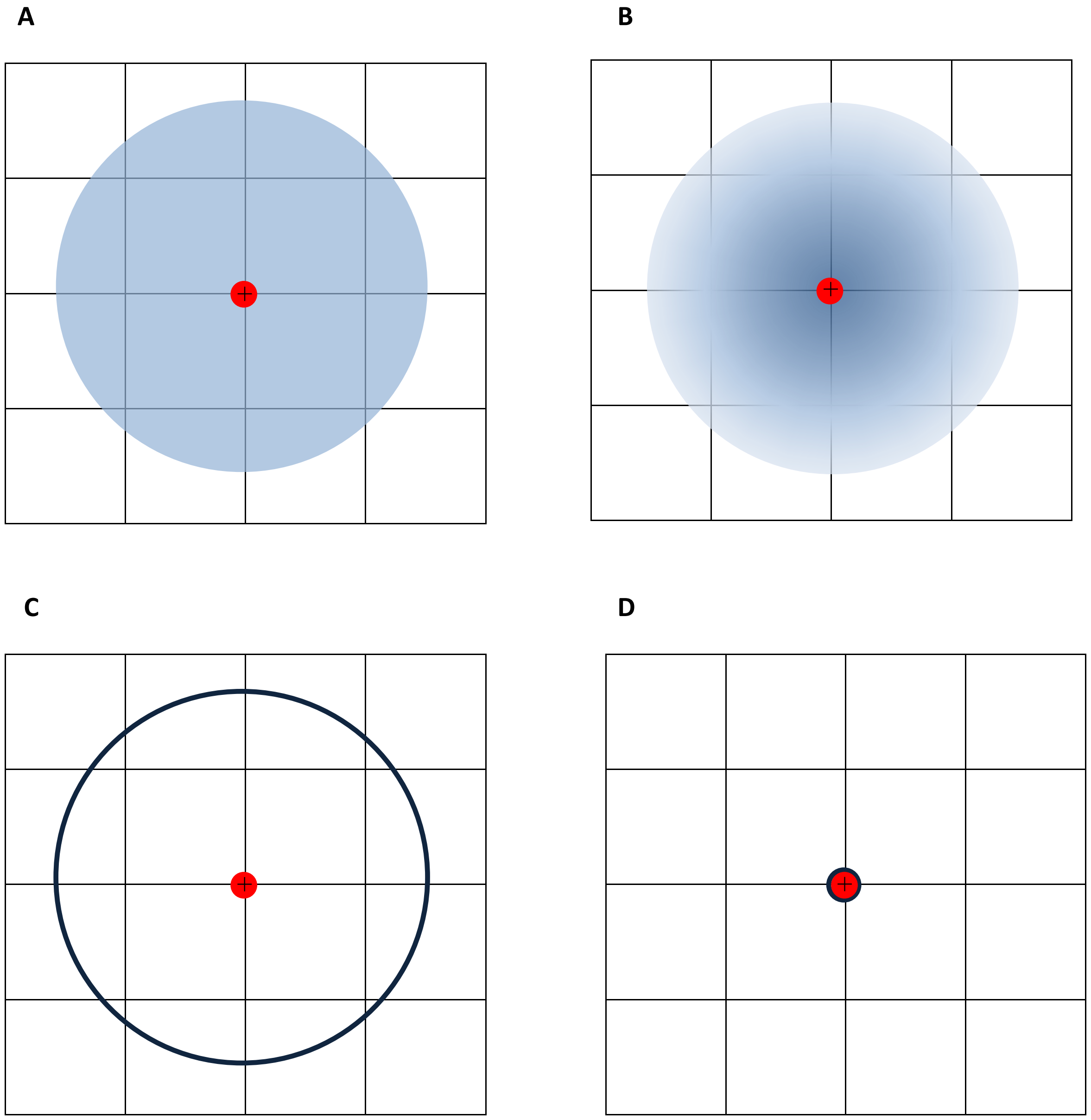


Figure 45: Exercise to facilitate conceptual change from the Bohr model to a concept of electron density.

In the following, students are asked about their expectations for the probability to find an electron around a hydrogen nucleus (see Figure 22). Students are also prompted to give explanations why other distributions are not realistic. Students' prior knowledge is typically activated strongly during that activity. Following classical physics, i.e. consulting Coulomb's law, option D would be the most favored one. But students know from previous encounters with atoms and pictures thereof that there must be some kind of shell (option C). If students combine what they know about atoms (there is a big sphere where the electron is located and a small nucleus) and the knowledge about Coulomb forces (the nearer the stronger the force) option B seems realistic. At that point, students are briefly told that strictly following classical mechanics (and Coulomb's law) the atom as we know it should not be possible and option D is what we would expect. However, such a distribution is not observed – for the moment students must accept this first discrepancy in the behavior of electrons inside an atom as a characteristic of the more complex quantum mechanics theory. The upside is, that with educated guesses and the use of prior knowledge (Coulomb's law and the existence of electron shells) the observed option can be guessed by about 40 % of students from the beginning. The aim is to show students: behavior in the quantum realm is not easy to predict, but still reasonable to some accounts.

At this point, the teacher will tell students that *Bohr's shell model* already explains some facts for single atoms (e.g. flame colors of different elements or ionization energy). However, this model reaches its limits when describing molecules, and is not suited to explain chemical bonds. It also contradicts modern quantum mechanics' idea that the position and velocity of an electron cannot be described with unlimited precision (Heisenberg's uncertainty principle). Thus, the concept of electron orbits is replaced by the idea that electrons have only certain probabilities of being located within a particular area. In the following *electron clouds*, i.e. a space in which there is a high probability to find an electron, are introduced. The *electron cloud model* has the advantage that the clouds are "deformable" and can "react" to more atomic nuclei. The probability to find an electron at a certain place changes with the addition of further atomic nuclei and electrons. With this model, the covalent bond can be better described.

As a next step students are faced with two approaching hydrogen atoms. They are asked to a) indicate attracting and repulsion forces (see Figure 46) and b) draw the expected electron density (see Figure 47). Note that the solutions and student guesses are already indicated in the illustrations.

Task 1: Use a green color to connect the electrically charged particles of the two hydrogen atoms that attract each other. Then, use a red color to connect those charged particles that repel each other.

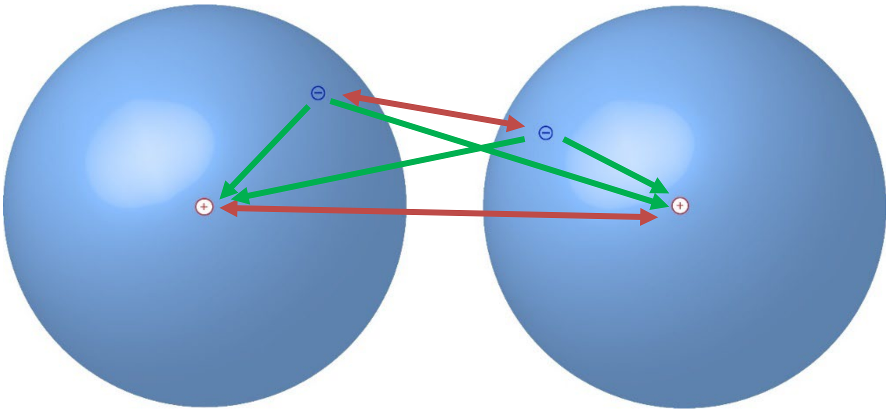


Figure 46: Student's task to indicate attracting and repulsion forces of two approaching hydrogen atoms. The forces in green and red are already indicated in this illustration.

Task 2: Where are the electrons more likely to be found in a hydrogen molecule (H_2) and where less? Draw an area where you would expect a high probability to find an electron.

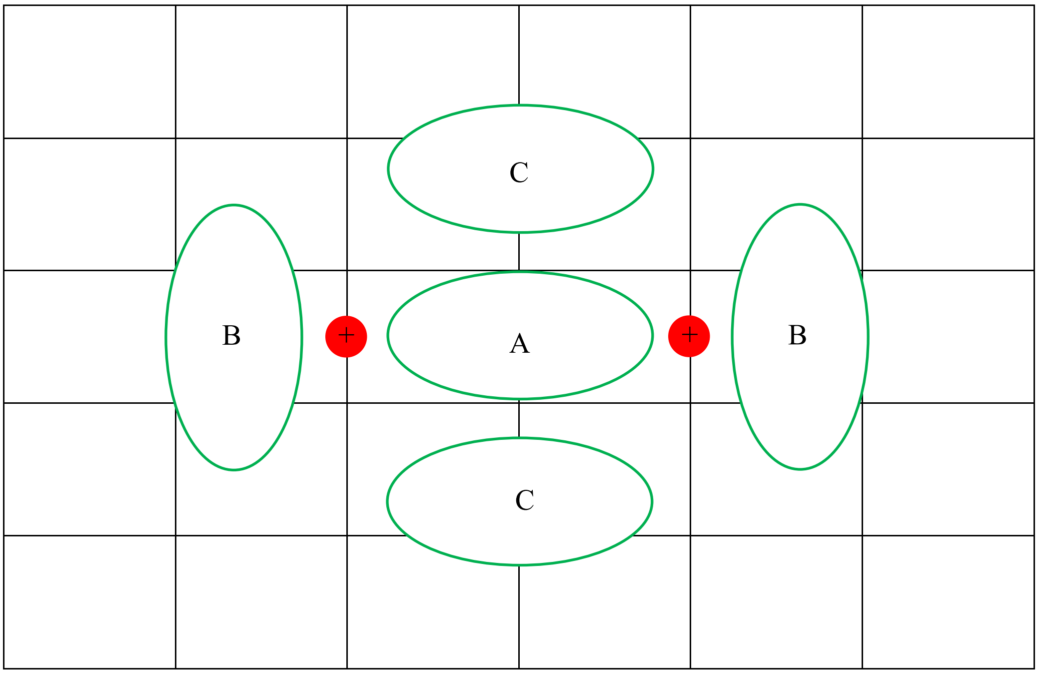


Figure 47: Students are asked to make guesses on the electron distribution in an H_2 molecule. Some students' guesses are already indicated in green (A-C) for a version without see appendix 3.

Students are asked to make educated guesses on how the electrons are distributed. Students' solutions are most interesting – some students will indicate the highest electron density in between the cores (A in Figure 47) to optimize the attraction of nuclei towards the electrons. Some students try to avoid close contact between electrons with the same charge (B) while others try to find a way how to implement both of those rationales (C). All of the above-mentioned proposals should be valued since they are grounded in valid thought processes.

Most students neglect the fact that the strongest attracting forces are still present close to the nuclei with a new probability of electrons being in between the two nuclei. Upon being presented with the observed probability (see Figure 48) students are told that the repulsion between electrons seems not to be observed – contrary to what one would expect according to electrostatic repulsion (Coulomb's law). Students are told for the second time that this is an important characteristic of the new model: Electron repulsion only occurs when there are more than two electrons present in a certain space. This is due to a property called *electron spin*. Without going into more detail students are told that electrons' behavior is as if they would not see each other. Compared to the single hydrogen atoms the probability of finding one of the two electrons has been changed. There is now a probability to find the electrons in between the nuclei. Such a doubly occupied electron cloud is called a *covalent bond*.

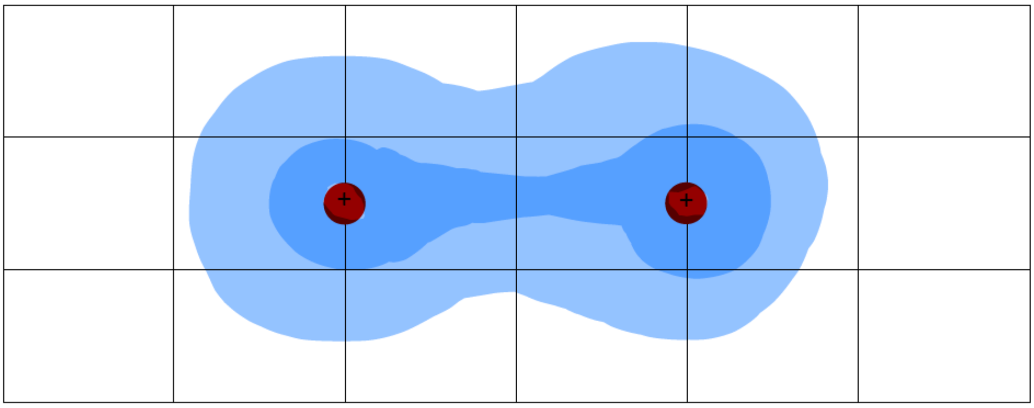


Figure 48: Teacher's hand notes of the electron density for a hydrogen molecule (H_2) with darker blue tones for higher probability.

When talking about diatomic molecules, like H_2 molecules, the Morse potential is normally introduced. It is sometimes also used to introduce covalent bonds in general. The Morse potential is a model to describe the potential energy in dependence on the distance between the two atoms. Typically, the aim is to show that there is a distance between the two atoms at which an optimum of attraction and repulsion forces is achieved – the bond length.

In this teaching unit, I invented an analogy to bring across the relevant points without actually presenting students with the potential curve. The analogy goes as the following: students are told that they should imagine that one of the two hydrogen atoms is located and fixed at the railway station while another hydrogen atom is on rails and driven in direction of the other hydrogen atom.

There are three different kinds of forces to consider when two atoms are approaching: a) the repulsion of electrons b) the attraction of electrons and atomic nuclei and c) the repulsion of atomic nuclei. Students are now asked to consider four cases (A – D in Figure 49) at different distances and to ask themselves which of the forces in play is dominant. At large distances, we expect the repulsion of the electron shells around the atom to be dominant – taking into account that in the case of two hydrogen atoms approaching this is not the case as has previously been stated (different spin state). The closer the atoms come the stronger the attraction of electrons toward both atomic nuclei (case B). When we look at two atoms in very close proximity (case D) we find that the repulsion of atomic nuclei is dominant. This leads to the conclusion that there must be an optimum between case B and D with equal attraction and repulsion forces as is indicated with case C. This distance is the optimum distance – the bond length. Any variation around this distance must be achieved with the upbringing of energy (either to counteract the repulsion of the nuclei or to counteract the attraction forces between nuclei and electrons).

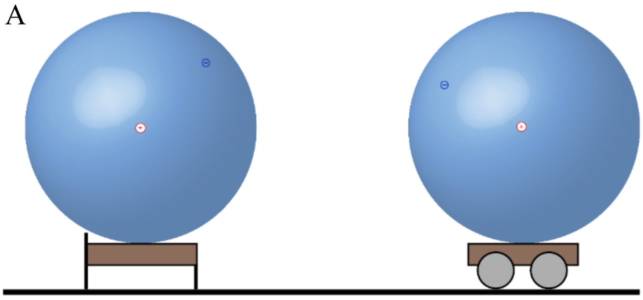
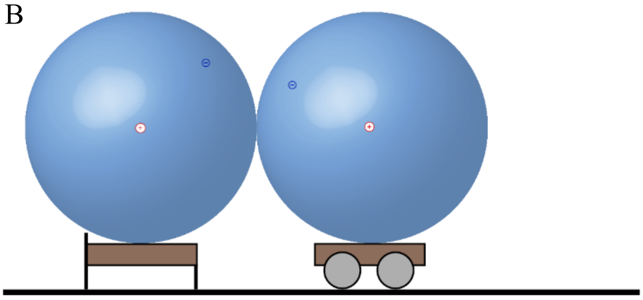
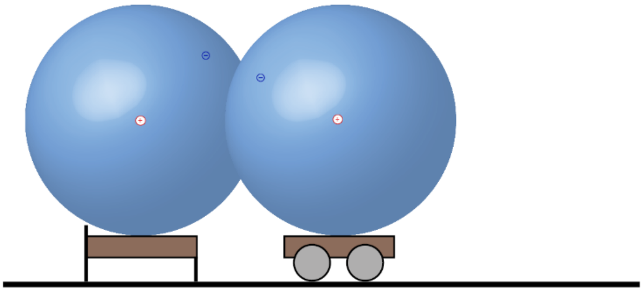
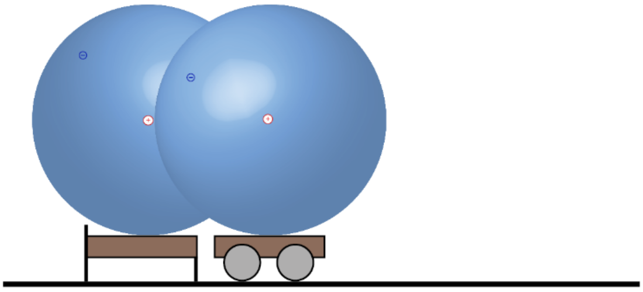
	Repulsion of the electron shells	Attraction of electrons and atomic nuclei	Repulsion of atomic nuclei
A 	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant
B 	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant
C 	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant
D 	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant	☐ Small ☐ Medium ☐ Large ☐ Very large ☐ Dominant

Figure 49: Train analogy for the approaching of two hydrogen atoms with the consideration of three forces: repulsion of electron shells, the attraction of electrons and nuclei as well as the repulsion of atomic nuclei.

Explicit Declaration of Heuristics with Further Rationalization

Heuristics is a powerful tool for educators in general. Unfortunately, they are sometimes used as explanations instead of declaring them as such. This can potentially lead to misconceptions and hinder conceptual change.

The Use of the Noble Gas Rule for the Explanation of Full or Empty Shells of Ions

Sodium (Na) reacts with chlorine gas (Cl_2) to yield sodium chloride (NaCl) in an exothermic reaction. In the formed sodium chloride crystals sodium is present as positively charged cations (Na^+) and chlorine as anions (Cl^-). The question for every chemistry educator is, how do we explain such chemical behavior? It is often the case that for this a simple heuristic is used: Sodium will give up its valence electron voluntarily to achieve the electronic configuration of a noble gas (i.e. neon). The problem with that explanation is the following: While it is of course true that the configuration is the same as the one of neon but it is not the reason why the Na^+ is formed. It takes energy to form Na^+: the first ionization energy is positive for sodium, i.e. the electron is not given up freely or voluntarily. When conducting the experiment one has to heat sodium with a Bunsen burner indicating that we need to activate the sodium quite heavily for the reaction to start. Only with sodium being heated up properly will the reaction with chlorine gas proceed. The formation of the salt crystal yields further heat that fosters the reaction.

The noble gas rule, a prominent and useful heuristic, is based on the shell structure of atoms (or the energy levels of orbitals). Atoms do not possess the will or a tendency to “be like a noble gas”. I am convinced that a proper distinguishing between heuristic and scientific explanations fosters conceptual understanding. But how can we explain such behavior without having to use quantum mechanical theory? To explain the charge of ions in ionic compounds knowledge of the shell structure of atoms as well as the Coulomb law is sufficient.

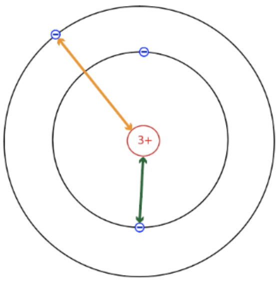
Students can easily follow that the inner electrons of sodium atoms are more strongly attracted than valence electrons in the outer shell. The low electronegativity of sodium atoms explains the fact that chlorine atoms can detach electrons from sodium atoms (easily to follow with the analogy of electron thieves and electron victims). With the following exercise (see
Figure 50) students understand why no more than all of the valence electrons of metallic atoms are taken and why non-metallic anions will only take up as many electrons as their valence shell allows for.

I propose that students are introduced to the simple rule of empty shells for metallic cations as well as full shells for non-metallic anions with such an explanation instead of relying on the noble gas rule.

Question 1: Metallic atoms are present in ionic compounds as ions that have given up all valence electrons. Can you use the Coulomb law to explain why metallic atoms keep electrons from inner shells?

The inner electrons of a cation are much more difficult to snatch by an electron thief than the distant valence electrons because of the shorter distance to the nucleus and the resulting higher Coulomb force.

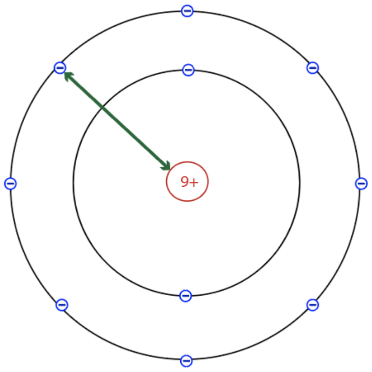
Ex.: Shell structure of the lithium atom



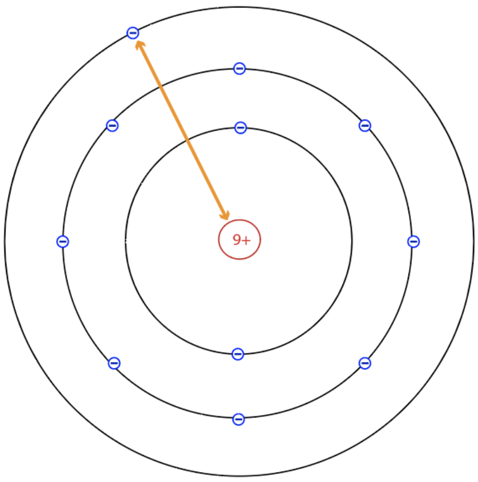
large distance to the nucleus

small distance to the nucleus

Question 2: Anions have full outer shells in ionic compounds. In the case of fluorine, this means that fluorine accepts another electron and forms an F^- anion. However, fluorine has the highest electronegativity of all the elements and is therefore one of the strongest electron thieves. Why can't the F^- anion accept another electron and exist as an F^{2-} anion? Consider the two anions in the shell model and argue with the help of the Coulomb law why an F^{2-} can easily become an F^- anion again.



F^-



F^{2-}

If we look at the F^{2-} anion in the shell model, we see that the electron that is farthest away from the nucleus is located on the most distant shell. This electron experiences a much weaker Coulomb force than an electron on an inner shell due to its greater distance from the nucleus. This comparatively low Coulomb force leads to the fact that this electron can be snatched away more easily, which results in the frequently observed F^- anion.

Figure 50: Exercise for students to understand the reason behind full- or empty valence shells of single atomic anions and cations in ionic compounds. Solutions are indicated in green.

The Use of the Noble Gas Rule for the Prediction of Lewis Structures of Molecules

The *noble gas rule* is also often used to explain the formation of molecules – some also call it the *octet rule* – referring to the fact that many molecules possess eight electrons (some of them shared with other atoms). Thereby students are led to the conclusion that the electronic configuration is always the same as one of the noble gases in the same period, i.e. typically eight or two valence electrons.

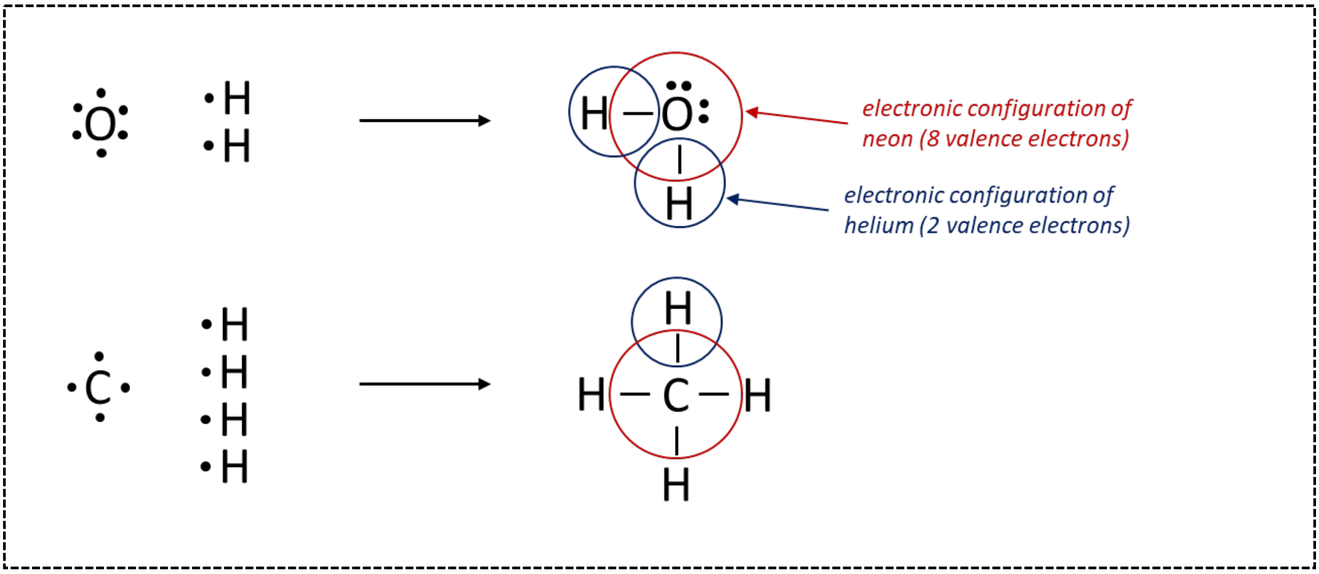


Figure 51: Illustration of the use of the noble gas rule to explain the formation of water (H_2O) and methane molecules (CH_4).

Theoretically, students can learn the rule without ever knowing anything about the nature of a covalent bond: two dots combine to form a dash (i.e. a covalent bond) and there cannot be more than four dashes around an atom (octet rule). While students are capable of drawing molecules and predicting the correct molecular formula of substances they might fail to actually understand what such lines represent. Additionally, there are known substances where this method fails: Sulfur hexafluoride (SF_6, Figure 52) for example is a very stable component used as an electrical insulator, Sulfuric acid (H_2SO_4) or its deprotonated form, the sulfate anion (SO_4^{2-}) are very prominent chemicals where the rules do no longer find appropriate application. Also, phosphoric acid (H_3PO_3) and its deprotonated form, phosphate (PO^{3-}), a common anion present in our bones and teeth, for example, cannot be described following this strict rule.

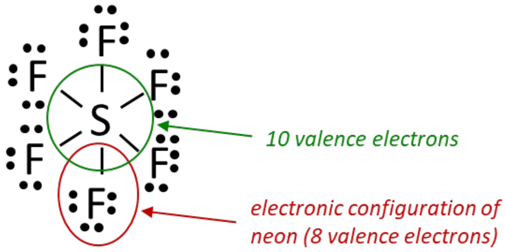


Figure 52: Lewis structure of sulfur hexafluoride (SF_6) with a hypervalent character that cannot be rationalized utilizing the noble gas rule.

The narrative of the noble gas electron configuration as a “desired configuration” by all elements is often supported by the inertness (or nobility in that sense) of noble gases. While all the noble gases do in fact exist as single atoms and some of them are used for their low chemical reactivity (e.g. argon as protection gas in chemical reactions) most of the noble gases can in fact form molecules. All of the heavier noble gases themselves (argon, krypton, xenon, and radon) do not follow the noble gas rule by building molecules: HArF, KrF_2, XeF_2, RnF_2 are described in the literature (Chernick et al., 1962; Fields et al., 1962; Grosse et al., 1963; Räsänen, 2014). The mentioned molecules form so-called three-center four-electron bonds (σ 3c–4e) first described as the *Pimentel–Rundle three-center model* (Pimentel, 1951). There are various hypervalent substances with great importance as potent reagents in organic synthesis, e.g. trifluoromethylation of organic compounds with the use of hypervalent iodine reagents (for an overview see Charpentier et al., 2015; or Zhdankin, 2013).

This raises the question of whether it is possible to introduce the underlying principle of the noble gas rule without the absolution it is usually taught with. In this teaching unit, I designed an approach in which students are led to the rule commonly known as the octet or noble gas rule but thereby leaving a door open for the before mentioned hypervalent structures (i.e. structures with more than four covalent bonds around a central atom). Students attempt to solve a task that is constituted as a productive failure (see Figure 53). The aim is on one hand to activate their prior knowledge and on the other hand to foster the awareness that the simple combination of two dots to draw a dash (i.e. a covalent bond) is not sufficient and that there are additional rules in place to be able to predict the correct molecular formula of substances.

Task 1: Make a suggestion for the structure of a molecule consisting of as many **atoms** of **H** as possible and …

a) … a **carbon atom** (C)
b) … a **nitrogen atom** (N).
c) … an **oxygen atom** (O).
d) … a **fluorine atom** (F).
e) … a **neon atom** (Ne).

Figure 53: Productive failure tasks for students to foster awareness for a maximum number of four doubly occupied electron clouds around a central atom.

After being introduced to how to draw Lewis structures students (e.g. one carbon atom with four hydrogen atoms, Figure 54; top) students are prone to simply follow the learned procedure and combine atoms to form NH_5 and OH_6 (Figure 54; middle and bottom). At that point, attentive students will start to suspect that something is not correct since students know from their daily life experience that the molecular formula of water is H_2O and not H_6O.

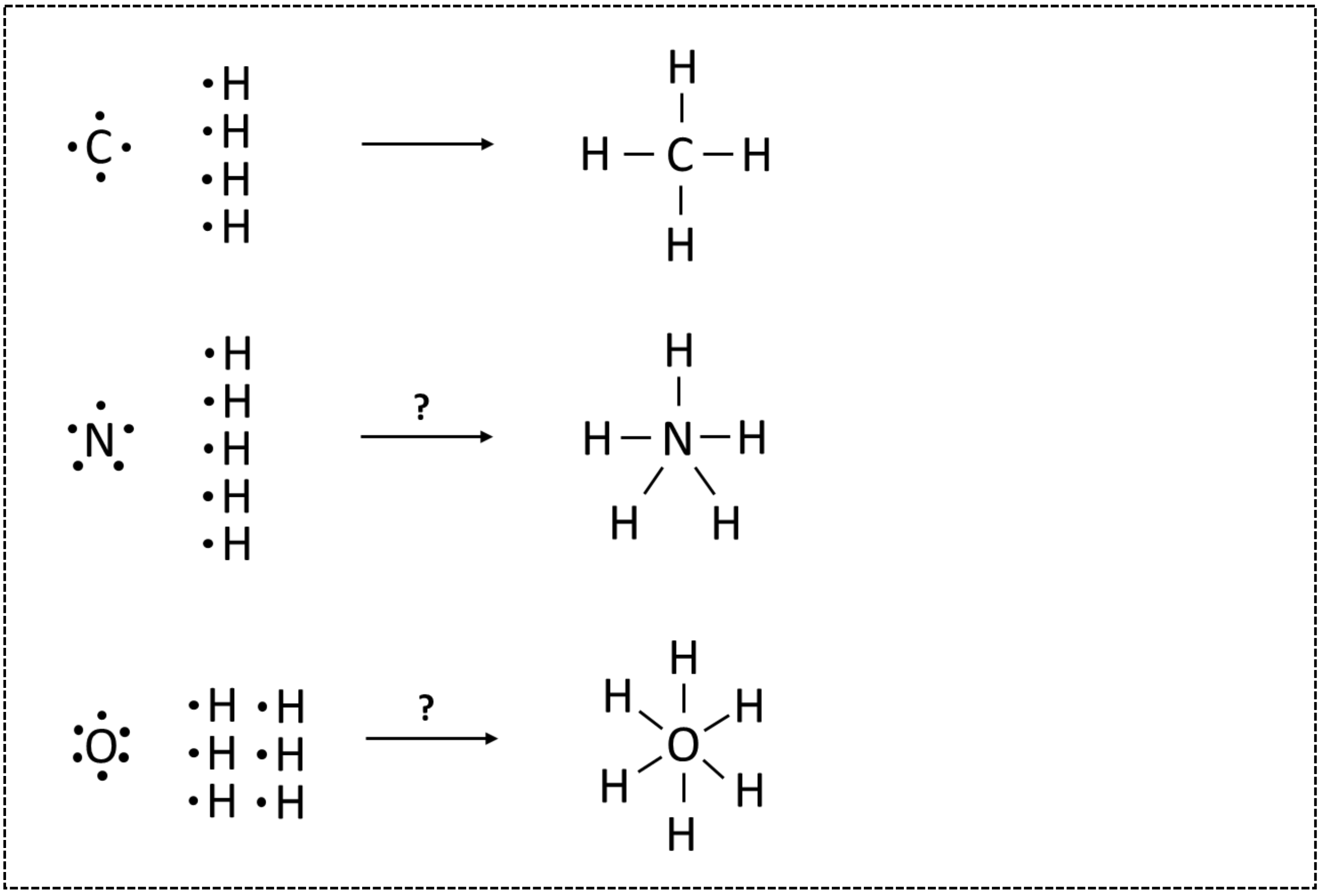


Figure 54: Following a simple procedure, i.e. the combination of two dots to form a covalent bond indicated with a dash, students will arrive at Lewis structures that do not correspond with molecules that are observed (NH_5 and H_6O).

At that point, students can be instructed on the existence of lone pairs (or non-bonding pairs), i.e. valence electrons forming a doubly occupied electron cloud which is less prone to combine with other atoms to build covalent bonds. The explanation given is a sterical hindrance, i.e. the repulsion of the doubly occupied electron clouds. An arrangement with six covalent bonds, i.e. six doubly occupied electron clouds, around a central oxygen atom is not observed (Figure 55, top). Typically, atoms of elements of the first two periods (elements hydrogen to neon) only form four doubly occupied electron clouds, i.e. covalent bonds or lone pairs, around the central atom. For an oxygen atom, this results in the formation of two lone pairs, with four of its six valance electrons, leaving two electrons to form covalent bonds with hydrogen atoms to form H_2O (Figure 55, bottom).

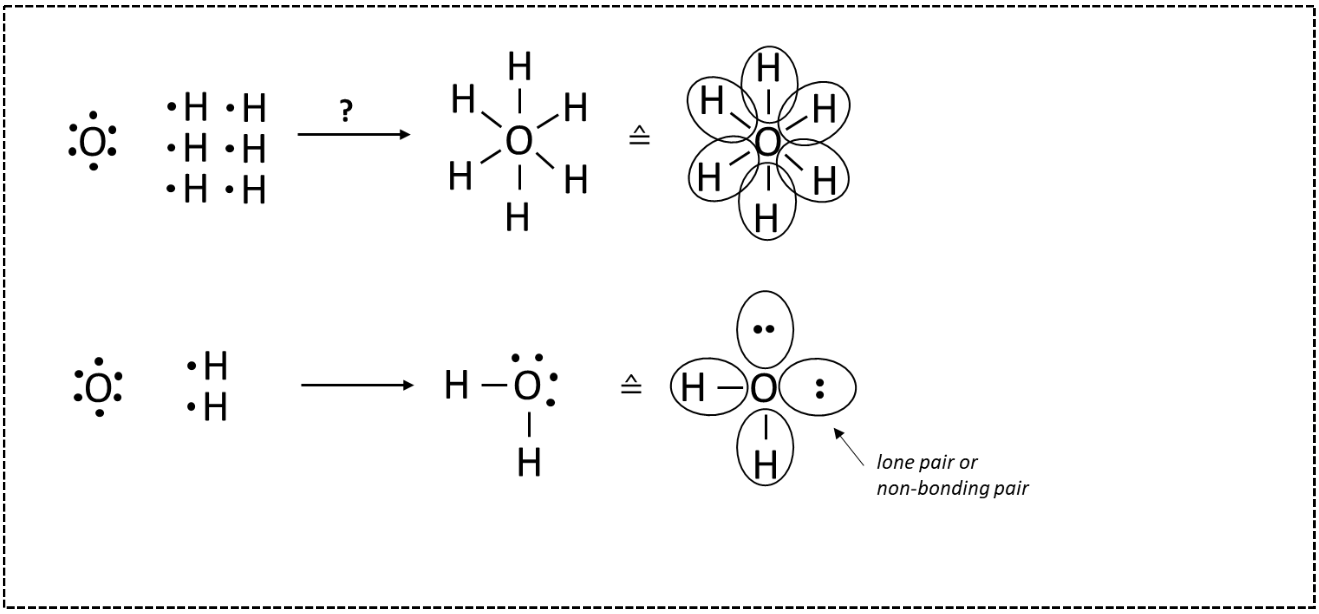


Figure 55: Explanation is given for students to understand the formation of lone pairs of oxygen atoms in a water molecule (bottom). Due to the repulsion of doubly occupied electron pairs around an oxygen atom H_6O is not observed (top).

This explanation has the advantage to result in the same heuristic but still offering the possibility for atoms of higher periodicity (e.g. sulfur, phosphorus) to form more than four covalent bonds around a central atom. If needed the explanation can be given at a later point, that atoms with more electron shells will form their covalent bonds farther away from the nucleus. This potentially allows for the formation of more than four doubly occupied electron pairs around a central atom. This explanation is still quite basic but allows for more complex molecules to be looked at. Furthermore, this explanation is in line with the possibility to introduce hypervalent molecules at a later point if needed.

After students have learned about the existence of lone pairs in some molecules they are prompted to apply their newly acquired knowledge by correcting their first proposal of the molecules in Task 1 (see Figure 53).

4.7 Fostering Students’ Awareness of the Differences between Intermolecular Forces and Chemical Bonds

Students have difficulties distinguishing between chemical bonds and intermolecular forces. Additionally, many students develop the misconception that intermolecular forces are present in metallic and ionic substances (see p. 48 for a more detailed discussion). The relative strength of chemical bonds and intermolecular forces is not clear to many students since typically the three bonding types are discussed as separate topics. The three types of intermolecular forces are conventionally taught after the covalent bonds, they might be compared to covalent bonds but most of the time the focus lies in the discussion of the relative strength of the intermolecular forces among themselves (dipole-dipole interaction, hydrogen bonding, and the Van der Waals forces).

But how can we efficiently bring across that *(4) “intermolecular forces are only present in molecular substances and their individual strength is smaller by several orders of magnitude compared to chemical bonds”*?

Explicit Comparison of Relative Strength of Intermolecular Forces with Chemical Bonds

Students encounter the intermolecular forces at the beginning of chapter 4 on covalent bonds for the first time in the reoccurring introductory experiment where the known bonding types are compared to each other (see chapter 4.6, p. 90). At that point, students are made aware of the pivot they might face when comparing melting points of different substances with the three types of bonds present: Ionic and metallic bonds need to be partially broken to allow for a change in physical state (e.g. from solid to liquid) for molecular substances that is not the case. Since the intermolecular interactions are smaller by several orders of magnitude those interactions are made obsolete when a system’s energy rises (e.g. by increasing the temperature). To sum it up: students are prepared for that very prominent misconception from the very first contact with intermolecular forces.

When students finally arrive at chapter 5 (intermolecular forces), students get the following task shown in Figure 56. They are asked to order various substances according to their boiling point. This task is set up as a partial productive failure: Typically, students are able to classify the substances by bonding type, by now students have learned that molecular substances have lower melting points than metals and salts. They might also be able to order metals and ionic compounds among themselves. But it is generally not possible to deduce the relative ordering of boiling points substances when metals and ionic compounds are compared. Additionally, students will fail in ordering the molecular substances according to their boiling point, because they lack the conceptual understanding of intermolecular forces. This exercise is constructed such that students activate their pre-knowledge (e.g. relative boiling temperatures of salts, metals, and molecular substances, procedural knowledge of how to order different metals and ionic compounds among themselves) and foster the awareness of the necessity to incorporate a new concept: The concept of intermolecular forces.

Task 1: Given the following substances:

MgO, H_2O, $NaCl$, CH_4, Cl_2, Al, N_2, Na, O_2, H_2

a) Try to classify these substances in ascending order according to their boiling temperature and justify your choice in each case.

Hint: Think about how the structure of the substances in each case. What does the boiling temperature depend on?

b) Can you match the substances to the given boiling temperatures (at standard conditions)?

Boiling temp. (°C)	**-253**	**-196**	**-183**	**-162**	**-34**	**+100**	**+882**	**+1465**	**+2470**	**+3600**
Substance										

c) Which substances are particularly difficult for you to classify?

Figure 56: Students are introduced to the concept of intermolecular forces with a productive failure task. Students are likely to activate their prior knowledge of the three types of chemical bonds and recognize their knowledge gap concerning intermolecular forces – the concept to be learned next.

Concluding remarks are the following: a) boiling temperatures of molecular substances are typically smaller than the ones of metals and salts, b) if molecular substances reach their boiling point intermolecular interactions are being weakened and broken (while covalent bonds are still intact).

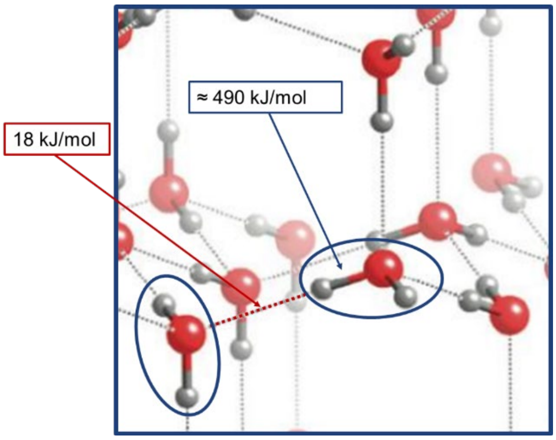
When asked about the state of evaporated water molecules many first-year ETH students showed difficulties: Students are made aware of the fact that the bonding forces in a molecule influence the general stability of the molecule and its *chemical reactivity* whereas the intermolecular forces influence the *melting and boiling temperatures* as well as the *miscibility* of molecular substances with other substances.

The explicit discussion of the great difference in individual strength of the covalent bond in a water molecule (blue in Figure 57) with the intermolecular interaction (hydrogen bonding, red in Figure 57) targets the observed difficulties students face when they have to distinguish between intermolecular and intramolecular forces, i.e. chemical bonds. Whereas the hydrogen bonding interaction of water is about 18 kJ/mol (Markovitch & Agmon, 2007), the covalent bond of a hydrogen atom to an oxygen atom is greater by several orders of magnitude (approx. 490 kJ/mol, Lehninger, Nelson, & Cox, 2005, p. 48). With follow-up questions, students are prompted to think about the consequences of the strength differences.

Differences between the Intermolecular Forces and Covalent Bonds

The **bonding forces** in a molecule have an influence on its stability and thus on the chemical reactivity of the substance.

The **intermolecular forces** influence properties such as the melting and boiling points, or its miscibility with other substances. They must not be confused with the bonding forces, i.e. the covalent bonds, between the individual atoms within a molecule.



Question: Can you explain why water is in the gaseous state at 100 °C, but its molecules stay intact at that temperature?

Figure 57: Comparison of the strength of the hydrogen bonding interaction between two water molecules (dashed, red line) with the strength of a covalent bond within a water molecule (blue). Illustration of the water molecules by Nick Greeves (n.d.) enlarged, labeled, and modified by the author.

Furthermore students are prompted to directly compare the relative strength of chemical bonds with the strength of intermolecular interactions (see Figure 58). Students are made aware of the fact that the strength of the different bonds can of course vary (indicated by the bandwidth of the bars in Figure 58) but that the intermolecular forces are generally weaker than chemical bonds. They are told that there are three types of intermolecular forces that are different in individual strength as well, indicated with light blue arrows in Figure 58.

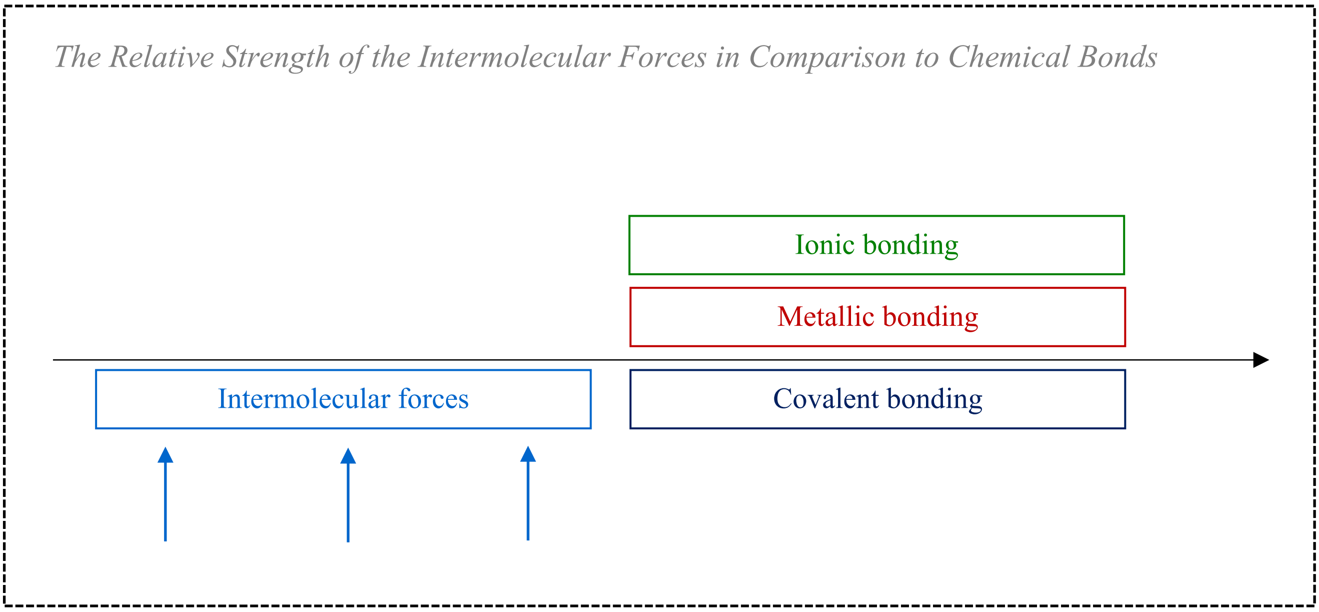


Figure 58: Illustration of the relative strength of the intermolecular forces compared to the three bond types. The bars indicate the bandwidth that can occur depending on the elements that constitute a substance. The three arrows indicate that there are three different types of intermolecular interactions.

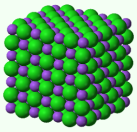
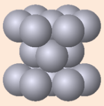
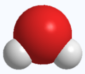
Highlighting the Inexistence of Intermolecular Forces in Metals and Ionic Compounds.

As has been described in chapter 2, many students hold the misconception of the existence of intermolecular forces present in ionic and metallic substances. The students are therefore explicitly told that this is not the case. The overview graph is extended to accommodate for the existence of the intermolecular forces (see Figure 59).

The Distinction of Intermolecular Forces from Metals and Ionic Compounds

Intermolecular forces are responsible for holding molecules together. However, the individual atoms of a molecule are held together by **covalent bonds**.

Metals are kept together by **metallic bonds** and ionic compounds by **ionic bonds.**

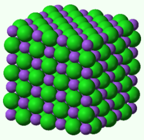
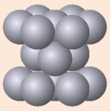
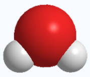
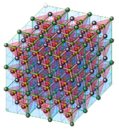
Type of Bond	Ionic bond	Metallic bond	Covalent bond		
Type of elements	Metal and non-metal	Metals among themselves	Non-metals among themselves		
Attraction between	Anions + cations	Atomic cores + electron gas	Atomic cores + electrons		
Types of particles or structures	Large ensemble of ions, forming an ionic lattice	Large ensemble of atoms, forming a metallic lattice	Small molecule		
Substance class	Ionic substances (salts)	Metallic substances (metals)			
Figures					

✗ ✗ **Intermolecular forces**

Figure 59: Extended overview table of the bonding types to accommodate for the existence of intermolecular forces. Students are made aware of the fact that intermolecular forces are not observed in metallic and ionic substances.

A direct comparison of the process of melting and boiling for different bonding situations should highlight once more that for ionic and metallic substances chemical bonds need to be broken while in molecular substances covalent bonds stay intact (see Figure 60). When heating molecular substances the weaker intermolecular forces are counteracted by the energy present at that temperature, i.e. the molecules stay intact but will no longer be closely held together as in the solid state.

Melting and boiling for different bonding situations

Type of Bond	**Ionic bond**	**Metallic bond**	**Covalent bond**		
Type of elements	**Metal and non-metal**	**Metals among themselves**	**Non-metals among themselves**		
Attraction between	**Anions + cations**	**Atomic cores + electron gas**	**Atomic cores + electrons**		
Types of particles or structures	**Large ensemble of ions,** forming an **ionic lattice**	**Large ensemble of atoms,** forming a **metallic lattice**	**Small molecule**	**Huge molecule**	**Large ensemble of atoms,** forming an **atomic lattice**
Substance class	**Ionic substances (salts)**	**Metallic substances (metals)**	**Low molecular weight substances**	**High molecular weight substances**	**Diamond-like materials**
Figures					

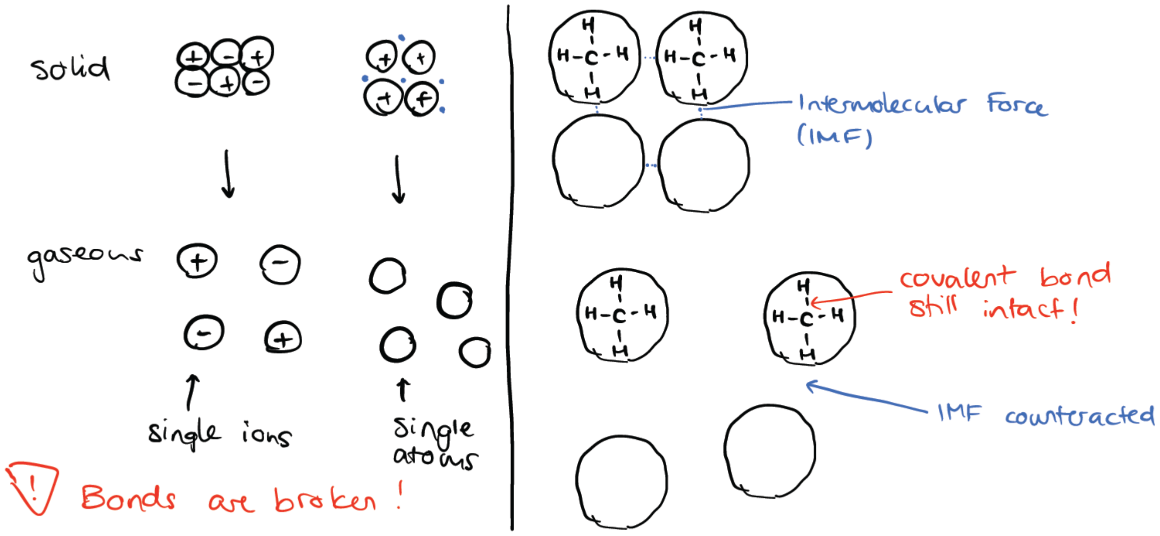


Figure 60: Teacher's hand notes of ionic, metallic, and molecular substances in the solid and the gaseous state. While ionic and metallic bonds are broken for a substance to be in the gaseous state, covalent bonds in molecular substances stay intact but the intermolecular interactions are no longer present in that state.

4.8 Fostering the Correct Usage of Chemical Bonding Language and the Targeting of Specific Misconceptions

Students use terms like molecule and lattice in daily life. It is a challenge for students to make themselves acquainted with the terminology used in chemistry classrooms. This project's investigations have shown that many first-year university science students still have a broad definition of the term *molecule*. Additionally, students have encountered the term molecule, without having had explicit chemistry education: prior knowledge with unspecific definitions of terms like *molecule* plays a vital role in the confusion students exhibit even after they covered the topic of chemical bonds in school. Additionally, the prominent misconception that all matter is composed of molecules needs to be addressed.

Chemical formulas play a vital role in chemistry education. Unfortunately, the information content that can be derived from the formula varies with the bonding situation present in substances. As shown in previous chapters the identified misconceptions associated with the term lattice need to be addressed as well.

The challenges described above are targeted by different means:

1. Refinement of terms used in daily language.
2. Fostering students' ability to correctly deduce information from chemical formulas.
3. Targeting observed misconceptions through self-explanations and holistic mental model confrontation.

Refinement of Terms Used in Daily Language

What does the term molecule mean? As described in more detail in chapter 2, p. 49 the term molecule is sometimes used inconsistently. This is an additional challenge for students to correctly understand the differences between the three bonding situations. It is my personal opinion that as an introduction to chemical bonding students should be made acquainted with a strict definition of the term molecule. This will help students see the difference between other bonding situations where no molecules are present. While even chemistry experts and some English textbooks on chemistry use the term molecule more broadly, in German-speaking parts the usage of the term molecule is typically handled more strictly. Students have prior knowledge about the term. Unfortunately, the definition in chemistry novices' minds is rather broad: They often assume that all matter is comprised of molecules and that it does not matter what kind of bond holds the atoms together.

1.Definition of the Term Molecule

A **molecule** is an atomic bond consisting of at least two non-metallic atoms linked together by covalent bonds.

Question 1: Use check marks (✓) if correct or crosses (**x**), if incorrect.

Chemical formula	Non-metallic atoms only	Covalent bond(s)	Uncharged atoms (no ions)	At least two atoms	If not a molecule: correct term
H_2	✓	✓	✓	✓	
NaCl	x	x	x	✓	salt / ionic comp.
Ar	✓	x	✓	x	atom(s)
H_2O	✓	✓	✓	✓	
CuZn	x	x	✓	✓	metal/alloy
LiF	x	x	x	✓	salt/ionic comp.
Fe	x	x	✓	✓	metal/atom

Figure 61: Narrow definition of the term molecule (according to German use of terminology) and a follow-up task to train students on the correct use of the term molecule. The solutions are indicated in green.

Yes, there are examples of organometallic molecules, and they are important but these are more or less special cases. I dare to say that when students have properly understood what a molecule is (in the strict sense), and what molecular ions are, then students will have no problem understanding more complex bonding situations. They will most likely also understand that an organometallic compound can be called a molecule since it shares the major attributes of a molecule: Most of the part of an organometallic compound is in fact of molecular character since the bonding situation is covalent. An argument can be made that even the attractive forces between a single metallic atom and the non-metallic atoms are of covalent nature. Therefore I advise that a more strict use of the term molecule would be helpful from the perspective of chemistry education. Many students show difficulties in distinguishing between different bonding situations, even after instruction on the topic. Why would we want to introduce a loose term which is used for the covalent bonding situation in a context where this is not the case? This approach is actively asking for misconceptions to foster. Realistically chemistry textbooks will not be changed so rapidly. Even some chemistry experts are using the term in an unspecific manner, which does not help the cause. I argue that when students have understood what the different bonding situations look like it is much less of a problem if they use the terminology more broadly.

Fostering Students' Ability to Correctly Deduce Information from Chemical Formulas

What can we deduce from chemical formulas? This is dependent on the bonding situation of the compound and the specific formula given. There are three kinds of chemical formulas: *molecular formula*, *empirical formula,* or *condensed formula*. Unfortunately, if it is not given explicitly, students can't easily deduce which one is meant since NaCl has similar surface characteristics as H_2O. More often than not students are left with a formula without knowing whether the formula is a *molecular formula*, an *empirical formula,* or a *condensed formula*. By first evaluating which bonding situation is present in the substance we can make further deductions on the information content we can derive from chemical formulas. To make this clearer to students I designed a task with exactly that goal (see Figure 62).

What information can be derived from a chemical formula?

In Chemistry classes, you often encounter chemical formulas. However, the meaning of the formula is not the same for salts and metals as it is for molecules.

Chemical formula	HCl	NaCl	NaK
Type of bond:	Covalent bonding	Ionic bonding	Metallic bonding
Presence of the smallest particles:	Neutral atoms/molecules	Na^+ and Cl^- ions	Atomic cores and electron gas
Term:	Molecule	Salt	Metal/alloy
The ratio of the elements contained:	1 H atom : 1 Cl atom	$Na^+ : Cl^-$ = 1 : 1	Na atoms : K atoms = 1 : 1
	The molecules are comprised of HCl, i.e. 1 H and 1 Cl atom.	No additional information (no NaCl molecules!)	No additional information (no NaK molecule!)

Conclusion: For metals and salts the chemical formula given is the empirical formula with information on the ratio of the elements contained. For molecular compounds, we can retrieve a piece of important additional information on the constitution of the molecule (therefore sometimes also called a molecular formula).

Figure 62: Exercise on the information content of chemical formulas depending on the bonding situation with concluding remarks. Solution and teachers' notes in green.

Chemical substances can be described via the chemical formula. For molecules, there are more sophisticated ways of how to draw chemical structures, e.g. Lewis structure or the skeletal formula for more complex molecules (see Figure 63). These tools are very important to efficiently bring across a lot of information on a molecule. The atoms are drawn in a two-dimensional fashion.

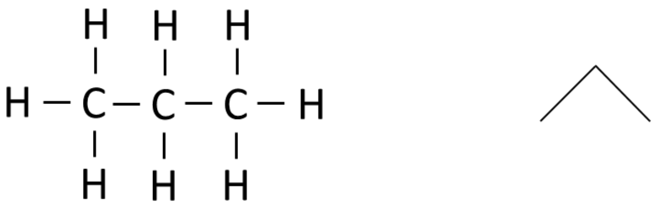


Figure 63: Lewis structure (left) and skeletal formulae (right) of C_3H_6

The molecules are three-dimensional and hence students need to make that inference themselves. To foster the understanding of the spatial arrangement of molecules, students deduce the tetrahedral arrangement of the covalent bonds around a central atom by themselves. Students are asked to find the best spatial arrangement of two doubly occupied electron clouds (blue in Figure 64) around a central atom (orange). The students are given six cases (A – E) and will deduce the best case by comparing the distances between electron clouds.

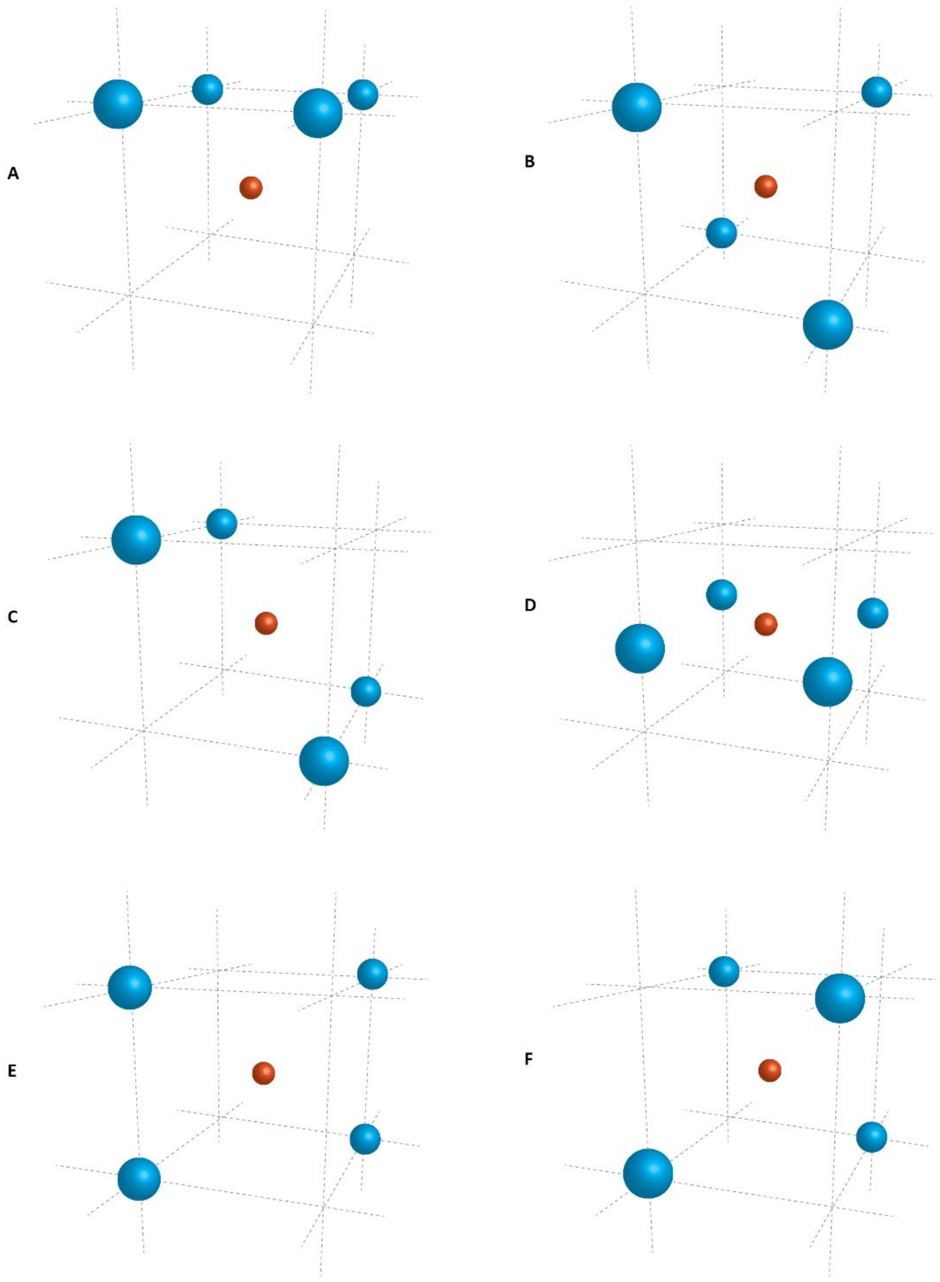


Figure 64: Inventing with contrasting cases task for students to find the best spatial arrangement of four doubly occupied electron clouds around a central atom.

When comparing different cases students are also actively targeting the misconception that molecules are flat as they are drawn in two dimensions on a piece of paper. Option D is a representation of this misconception. Students are therefore asked to compare the distances and realize that in the case of D the distance between electron clouds is the length of the cube's side (red line in Figure 65). In the case of F, i.e. the tetrahedral arrangement, the distance is the diagonal of the cube (green line in Figure 65). This exercise is aimed at fostering students' ability to understand the tetrahedral arrangement of molecules like CH_4.

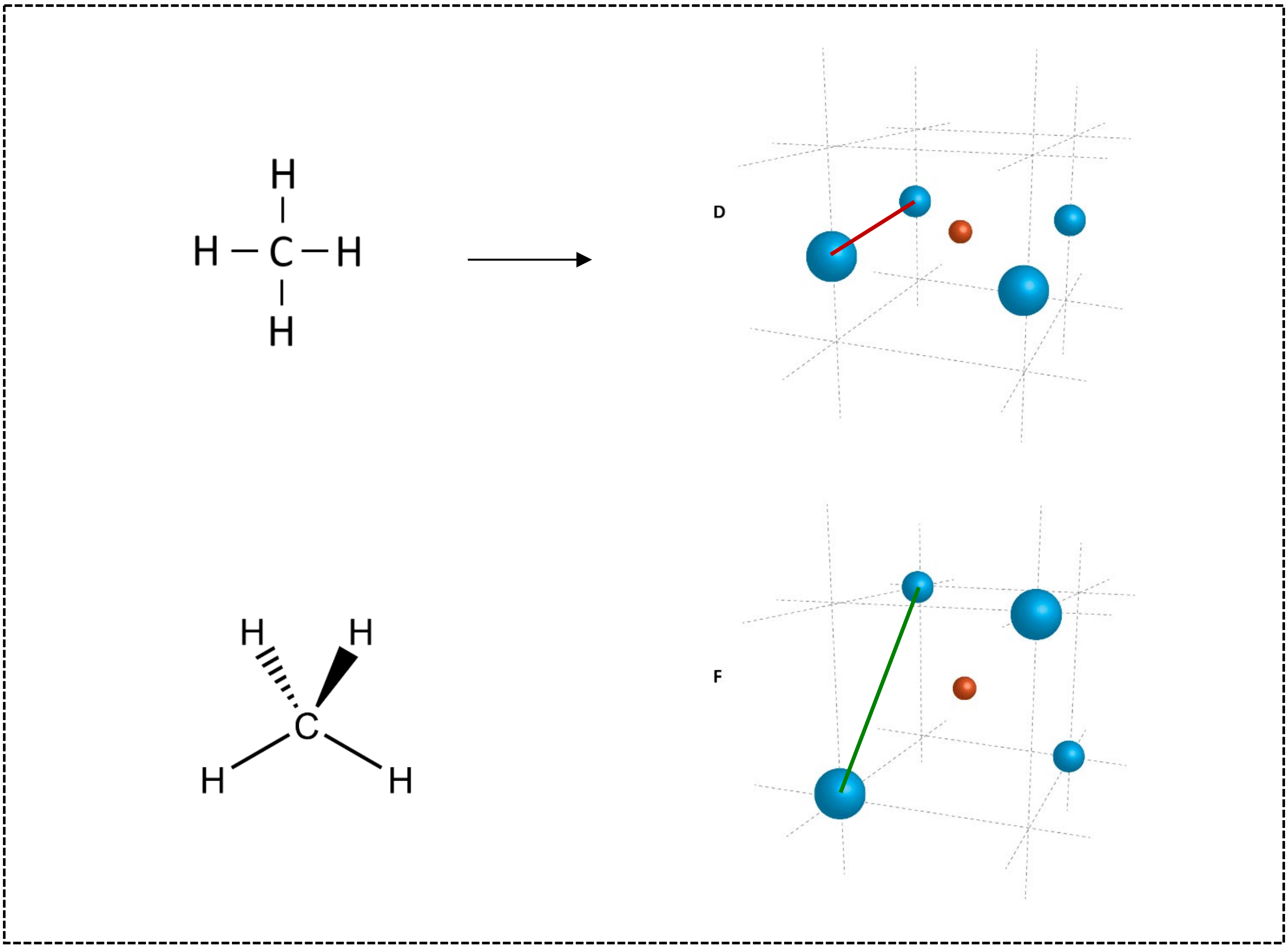


Figure 65: Explanation for students to understand why the planar arrangement of doubly occupied electron pairs is not observed: While for case D all the distances between the doubly occupied electron pairs is the length of the cube's side (red line) the four distances for the tetrahedral arrangement (case F) are the diagonals of the cube (green line). This explanation sets the basis for the introduction of the Natta projection (bottom left).

This exercise lays the foundation for the introduction of the more precise *Natta projection* (bottom left; Figure 65) and the *valence shell electron pair repulsion theory* (VSEPR). Using this relatively simple theory students can predict the three-dimensional arrangement of molecules.

Targeting Observed Misconceptions through Inventing with Contrasting Cases, Self-explanations, and Holistic Mental Model Confrontation

Various misconceptions revolving around the idea of molecules have been identified by an assessment conducted within this dissertations project:

1. Unspecific use of the term molecule
2. All substances are comprised of molecules
3. There are sodium chloride molecules (with various synthetic variations of the misconception) and/or ion pairs in molecules.

How can we actively target such deeply rooted misconceptions that seem to persist to exist even after being instructed on ionic compounds in length at the Gymnasium level? Previous work has shown great promise for the use of self-explanations (for an overview see Fiorella & Mayer, 2016; Wylie & Chi, 2014) and holistic mental model confrontation (Gadgil et al., 2012) to actively target misconceptions. An introduction using inventing with contrasting cases targets the misconception of the ions paring at the beginning of the introduction of the ionic lattice structure.

Inventing with Contrasting Cases for the Deduction of the Ionic Lattice Structure in Ionic Compounds

As has been described in chapter 2, the misconception concerning the idea of ion pairs in ionic compounds is common. To target the misconception, an inventing with contrasting cases task has been developed: Students are asked to compare four different arrangements of ions (see Figure 66). It is important to add the note that students should also argue against the other options since the correct answer is relatively easy to spot for students. The process of ruling out the arrangements that do not occur in an ionic crystal is as important as the finding of the actual arrangement. While option C can be ruled out very easily (repulsion of ions with the same charge) options D and B are harder to argue against. In the case of D, students should be made aware of the fact that there are no repulsion forces and this arrangement is not generally unfavorable. This arrangement would not explain why we can see ionic crystals by eye: We would never be able to see such a fine line of ions. Additionally, it must be argued with the Brownian motion that at room temperature ions will be in motion. This automatically leads to arrangement B after a while – like a rope that is brought into motion. This fact can be made more salient to students with the use of a physical magnet model: While electrostatic attraction is not the same as magnetic attraction, many principles are similar (two poles, same polarization leads to repulsion, different polarization leads to attraction, the closer two magnets the stronger the force). With this model the before described folding of an ionic “string” to form the arrangement B can easily be shown. Option A is harder to argue against. The Brownian motion argument can be made as well: Two of such ion pairs would still attract more ion pairs leading to arrangement B in the long term. Additionally, such an arrangement will never be visible to the eye and looks more like sodium chloride in the gaseous state. At this point, it should be stressed that such ion pairs are not formed in an ionic crystal. They might be formed in the gaseous state of ionic compounds under certain conditions, but we do not observe such pairing in a sodium chloride crystal for example.

Question 1: The goal of this question is to think about how positively and negatively charged ions will arrange themselves when brought together. Which of the following graphs do you think best represents the expected arrangement? Circle it and explain why you chose it and why you ruled out the other options.

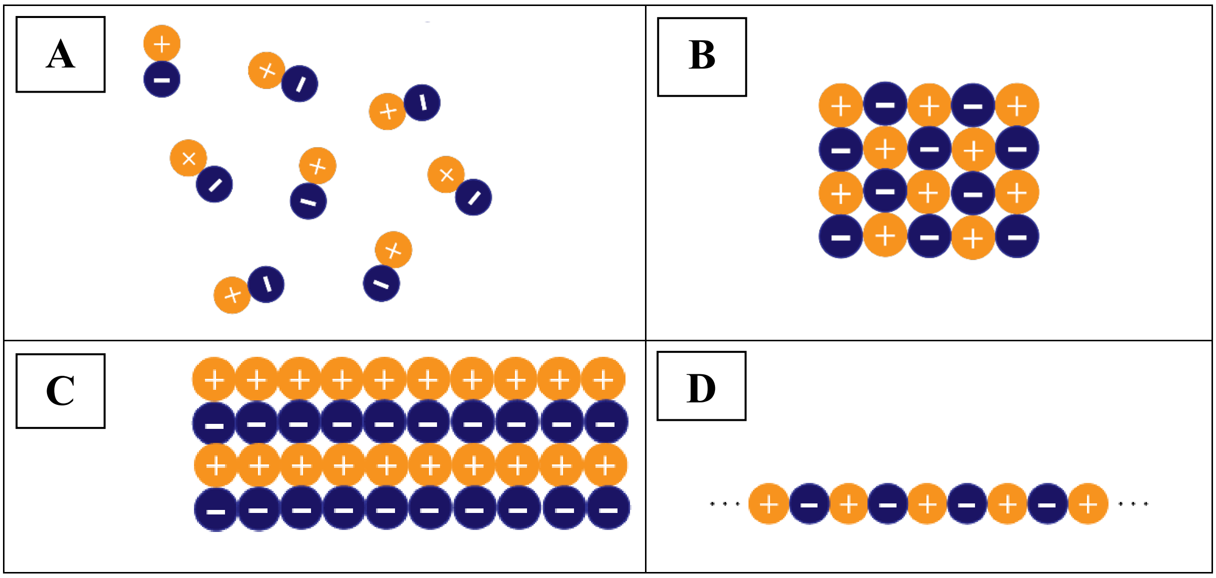


Figure 66: Inventing with contrasting cases task about the formation of ionic lattices and ionic pairs.

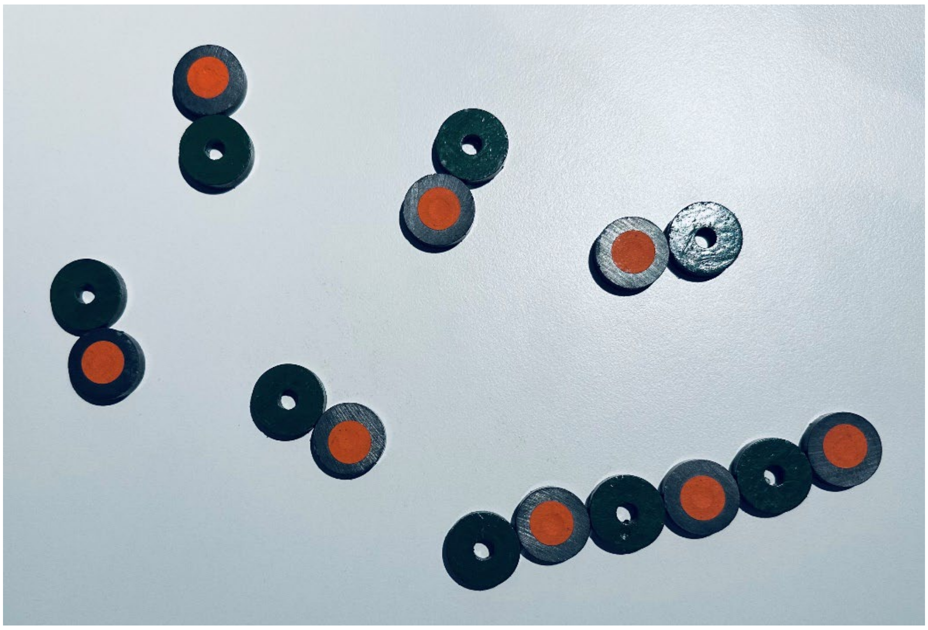
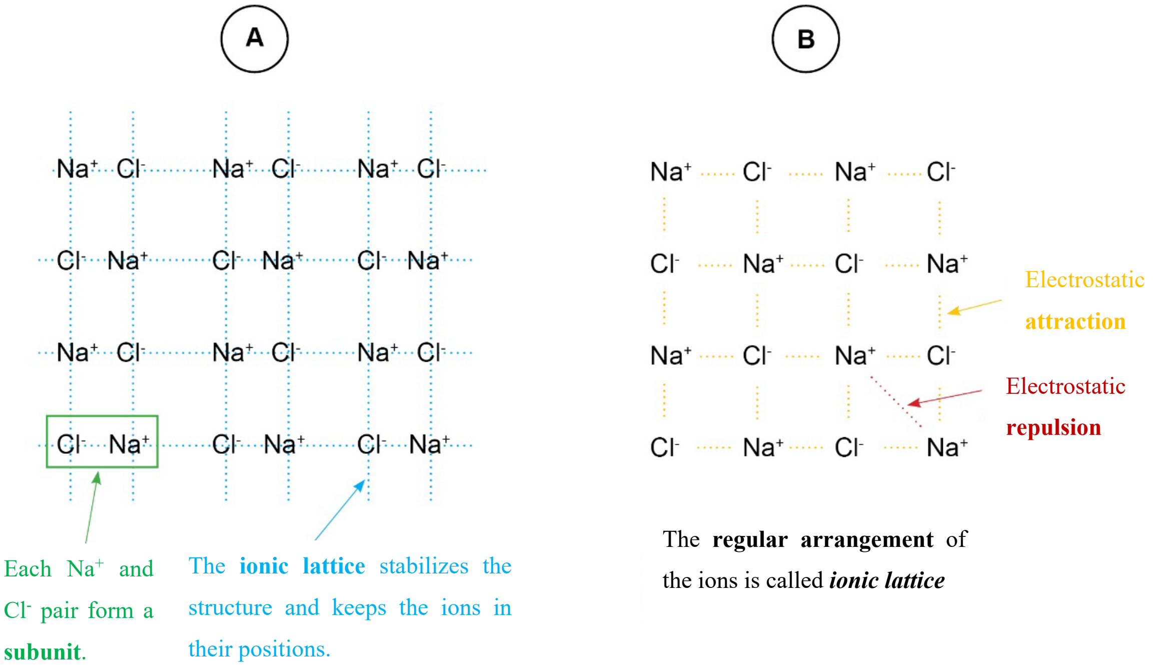


Figure 67: Use of the magnetic model to argue for and against the arrangement of ions of a salt crystal. A B C D

Holistic Mental Model Confrontation

The misconceptions concerning the existence of molecules in sodium chloride are various. Additionally, many students think of the lattice as something strong and physical (see p. 50). To tackle such misconceptions is a challenge: One possibility that makes use of the positive effects of comparing and contrasting activities is the holistic comparison of two mental models. This method has first been described by Gadgil et al. (2012). Thereby many misconceptions are built into the faulty model A (see A in Figure 68) and compared to the expert model B. This has been shown to foster conceptual change even more efficiently than self-explanations (Gadgil et al., 2012). It is important to focus on the similarities as well as the differences between the models, therefore students are prompted with follow-up questions to guide their attention to those aspects.

Question 1: Two models of a common salt crystal (sodium chloride, NaCl) are shown below. Compare the expert model B you learned in class with the faulty model A and answer the following questions.



Each Na$^+$ and Cl$^-$ pair form a **subunit**.

The **ionic lattice** stabilizes the structure and keeps the ions in their positions.

Electrostatic **attraction**

Electrostatic **repulsion**

The **regular arrangement** of the ions is called ***ionic lattice***

a) What are the similarities between model A and expert model B?

b) How does the expert model B differ from model A?

c) Which aspects are misrepresented in model A?

Figure 68: Holistic mental model confrontation of a faulty model containing many misconceptions (A) with the expert model (B).

Use of Different Kinds of Physical Models Representing a Sodium Chloride Crystal

Misconceptions concerning ionic lattices have been documented for first-year students before attending lectures at university (see *university evaluation studies 1 and 2*, chapter 2). Ions are arranged in an ordered manner: The symmetry of ionic compounds allows for the repetition of the so-called *unit cell*. The symmetrical arrangement of ions is described as the *ionic lattice*. The Lattices chemistry educators talk about do not exist as physical entities in ionic crystals. Unfortunately, there are physical models of ionic compounds with metal bars between the ions potentially fostering the described misconception (right in Figure 69). There are also closed-packed models now available making use of balls with magnets on the edges (left in Figure 69).

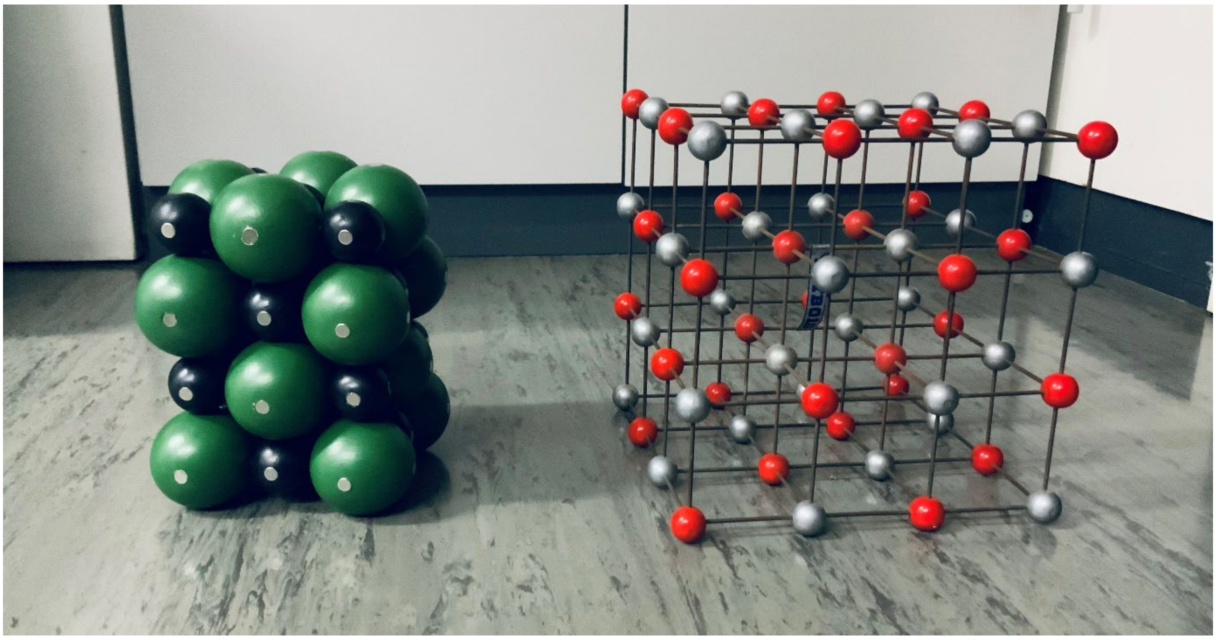


Figure 69: Photograph of two models of sodium chloride: left model with the closed-packed arrangement of ions (left) and model with large spacing between the ions and metal bars to hold the balls representing ions together (right).

Self-Explanations as a Tool to Foster Conceptual Change

Besides the use of holistic mental model confrontations as well as the use of different kinds of physical models, what can be done to foster the correct understanding of ionic lattices? Self-explanations have proven to foster conceptual change in various settings (for an overview see Fiorella & Mayer, 2016; Wylie & Chi, 2014). We therefore also implemented self-explanation tasks to tackle the most prominent misconceptions discovered while assessing first-year university students' understanding of chemical bonds. An example of such a self-explanation task is found in Figure 70. Students are asked to help out Hugo, who is holding on to typical misconceptions about ionic lattices. Self-explanations can be used in different ways, in this case, the student's task is concentrated around a common misconception. The advantage of such a self-explanation task formulated in the described manner is that students a) confront their own or similar misconceptions and b) are made aware of their gaps in knowledge on the topic.

Question 2: Hugo is outraged by the teacher's explanation that the ion lattice in salts does not occur as a physically existing lattice that holds the ions in their positions.

a) Explain to Hugo the reason why the ions stick together and are hardly movable at room temperature.

b) Explain to Hugo why the term "lattice" is used by telling him exactly what the ion lattice describes.

Figure 70: Self-explanation task about ionic lattices: By formulating explanations students confront their misconceptions in case they hold on to those and get feedback on possible knowledge gaps.

5 Evaluation of the Comparing and Contrasting Teaching Materials in Upper Secondary School

5.1 Research Questions

The *university evaluation studies 1 – 2* revealed a severe lack of understanding of chemical bonding even in very selective groups of science students (see chapter 2). The identification of the major challenge, overgeneralization, and common misconceptions laid the basis for the development of a new teaching unit (see chapter 4). The method of comparing and contrasting was chosen as an appropriate method to tackle the observed challenges (see chapter 3 for the reasoning of this choice). Therefore, the teaching materials contain many comparing and activating activities and focus on comparing the three different bonding types from the very beginning (see chapter 4 for a detailed description of the teaching materials). The chemical education research community has so far not investigated the effectiveness of such an approach. Therefore, the main research questions of the *Gymnasium intervention study* were:

1. Does the comparing and contrasting teaching material foster the conceptual understanding of chemical bonding more strongly than conventional instruction?

2. Do students, instructed with the comparing and contrasting teaching materials, show lower frequencies of misconceptions at the follow-up test, three months after the intervention, compared to a control group instructed on the topic with conventional teaching material?

5.2 Brief Overview of the Study Design and Hypotheses

The study was set up as a pre-post-test classroom intervention study at the Gymnasium level with two groups: An *intervention group* and a *control group* (see Figure 71 for an overview). The intervention group was instructed with the comparing and contrasting teaching materials, whereas the control group was taught with the materials the teachers have been using so far, i.e. conventional teaching materials which are characterized by sequential instruction.

To assess students’ prior knowledge, a pre-test (CBI pre-test, see chapter 2.4) was applied in the lesson before the instruction on chemical bonding started. In the following, students were taught with the developed teaching materials using many comparing and contrasting activities (intervention) or with conventional teaching materials, following a more sequential method of instruction (control group). Immediate effects (post-test), as well as long-term effects (follow-up) three months after the instruction on (1) the conceptual understanding and (2) the frequency of misconceptions, were investigated.

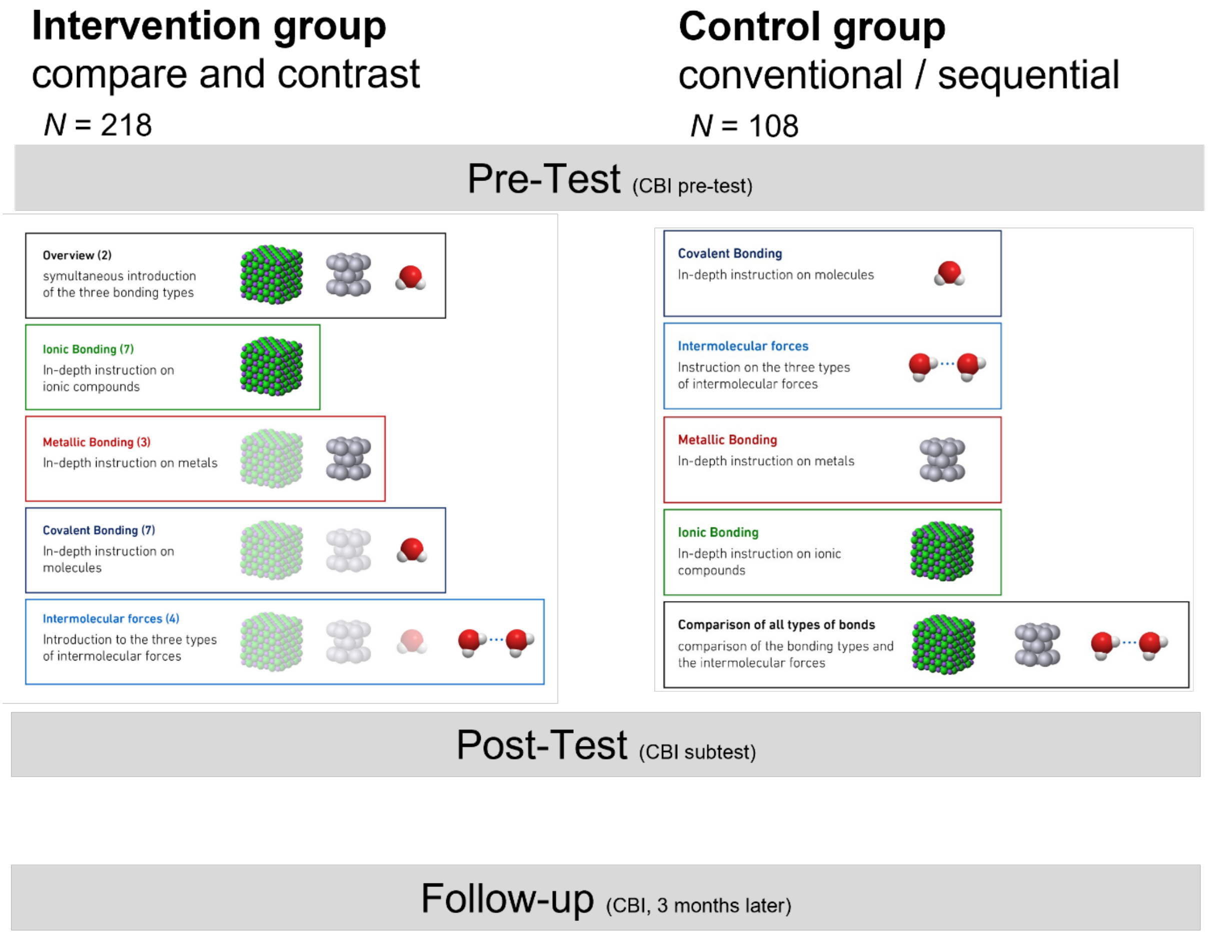


Figure 71: Design of Gymnasium intervention study with pre-test, post-test, and follow-up. Note: pre-test differs from post-test and follow-up (7 link items)

Hypotheses

The simultaneous introduction of concepts is more demanding for students than the sequential introduction. This might result in desirable difficulties, which are cognitively activating (Bjork, 1994), or in cognitive overload, which is detrimental (see chapter 3.2 for a more detailed discussion). The method of comparing and contrasting has not been investigated for its application for the instruction of chemistry topics in general, and chemical bonds in particular. The idea behind comparing and contrasting is in theory very much applicable to the topic and the aforementioned difficulties. Hence, my hypotheses were the following:

Hypothesis 1: The intervention group outperforms the control group at the post- and follow-up test on conceptual understanding.

Hypothesis 2: The intervention group's frequency of misconceptions is lower than in the control group three months after the instruction on chemical bonds.

5.3 Methods

The study was conducted with 15 10th-grade classes and eight different chemistry teachers from five different Gymnasium schools in the German-speaking part of Switzerland. The Gymnasium is the highest track of the public school system in Switzerland providing high school and secondary education to students with high achieving scores in primary school. About 20% to 25% of all primary school students in Switzerland attend the Gymnasium from age 12 to age 19. With the completion of the Gymnasium track, students acquire the diploma (Matura) which allows for entry to all Swiss universities. Students participating in my studies were recruited via teachers interested in participating in the study.

The Teachers

Teachers were recruited via a chemistry teacher training program at our university. Experienced chemistry teachers who provide practice lessons to aspiring chemistry teachers were asked to participate in the program. They are skilled in their profession and possess at least five years of teaching experience. Three teachers were willing to participate in the first year of the study (in the school year 2020 – 2021) and another five in the following year (2021 – 2022). At this point, I was evaluating the teaching materials for their practicality in a real classroom setting. Hence, I was one of the teachers of the first round of investigations (see section 4.2 for the development and optimization of the teaching materials). Five of the eight chemistry teachers involved in the study were teaching a parallel class of the same age at the same school. This allowed for stronger control of the teacher's effect on the study: Every teacher providing a class for the control condition also provided a class for the intervention condition. The assignment of one of the two parallel classes to the intervention or control group was done randomly. The initial goal to recruit chemistry teachers with parallel classes was not met for three teachers (one being myself) because they were unexpectedly not assigned a parallel class in this school year. Those teachers were assigned to the intervention group. Two additional teachers were interested in the study but could not be included because they could not finish the intervention due to health reasons and classes being taken over by different teachers.

Student Sample

Gymnasium students were recruited indirectly through teachers interested in my research project. Since the study was conducted in a regular classroom setting, classes could not be separated into randomized groups. The groups are therefore nested in classes. Every participant was informed about the study and the tests to be performed as well as the data to be collected and then asked to fill out a consent form for the allowance of usage of their data (see appendix 2). The data was collected anonymously with a student-generated code (see the first page of tests, e.g. appendix 1.1) in accordance with the ETH Zurich Ethics Commission (see appendix 2, EK-2021-N-123). Students who did not approve of the usage of their data would of course still be part of the classroom and also fill out all the tests without being analyzed and utilized for scientific purposes (5 cases in total). The classes were rewarded CHF 200 for participation (regardless of intervention or control) in the study and students were informed that they would have the possibility to see how they performed after the intervention by reconstruction of their personalized code. Students were also informed that their performance in the intervention did not influence their school grades.

The final *Gymnasium intervention sample* consisted of 326 Gymnasium students (205 female, 116 male, 8 diverse, mean age 16 years, grade 10), grouped in 15 classes, taught by 8 different teachers. Four of the 15 classes were taught in English (immersion classes) equally distributed between control and intervention conditions. The classes have not been instructed on chemical bonding before. Two classes could not fill out a follow-up test because the students were on a postponed language exchange in England for three months. The intervention group was larger (218 compared to 108) because some teachers interested in my research did only have one class to participate in the study. With those classes assigned to the intervention group, the number of classes being part of the intervention grew larger.

Measures

To assess the *conceptual understanding* of chemical bonding models, as well as the frequency of misconceptions in this context, the chemical bonding inventory (CBI) was used. At the post-test, the previously described CBI subtest was used, and at the follow-up test, the complete CBI was administered (see chapter 2.5, p. 53 for an overview of the tests used in the empirical studies).

Conceptual Understanding of Chemical Bonding Models

The main goal of this investigation was whether the developed teaching materials foster conceptual understanding to a greater extent compared to conventional instruction. Hence an appropriate assessment tool or inventory was required. Since no such assessment tool was accessible or described in the literature, I had to develop the *Chemical Bonding Inventory* (CBI, see chapter 2 for a review of existing inventories and the development of a new inventory). The CBI was originally designed to evaluate students' conceptual understanding of bonding before beginning their studies at university but could also be used for this intervention study. The CBI laid the basis for the assessment of conceptual understanding directly before (pre-test), immediately after (post-test), and three months after the intervention (follow-up). All tests were administrated as pen-and-paper tests.

As described in chapter 2.4 in more detail, it was not possible to use the full CBI as a pre-test due to insufficient understanding of terminology, instead, the *CBI pre-test* was used. Seven items from the

CBI were used as link items, i.e. items present in pre-, post-, and follow-up tests. To assess prior knowledge appropriately, 11 items covering the topics of the *structure of atoms* as well as *Coulomb's law* were designed. Those additional items evaluated the understanding of concepts that are needed to build upon to better understand the interaction between atoms and ions, i.e. chemical bonds.

At the post-test, the *CBI subtest,* and at follow-up, the complete *CBI* was administered (see 2.5 for an overview of the tests used in the empirical studies). The follow-up and post-test were hence very similar: All items of the post-test (maximum score of 25) are also present in the follow-up test (maximum score of 31) except for the in-depth evaluation of the understanding of intermolecular forces (Q23 – Q25). Since the developed teaching unit only gives a brief introduction to intermolecular forces items, students were not expected to be able to solve items Q23 to Q25. At follow-up, three months after the intervention students could be expected to solve the items, since intermolecular forces were covered in class in the meantime. The follow-up test contains the same items as the developed inventory on chemical bonding I developed and assessed in the *university evaluation studies 1 – 2*. For the reason of better comparability of post and follow-up tests only the follow-up score containing common items (i.e. the CBI subtest, Q1 – Q22) is described as the follow-up total score in the following (maximum points = 25). Items Q23 and Q25 are only used for the calculation of the frequency of misconceptions (see below).

Frequency of Misconceptions

As described in more detail in chapter 2, a measure for the evaluation of the prevalence of misconceptions was used: the *frequency of misconceptions* (FoM) (see p. 27 for an example). Single incorrect answers pointing towards the prevalence of a certain misconception were counted and added up for all items of the CBI resulting in a mean score for every misconception. Dividing by the total number of distractors taping into this misconception, a *frequency of misconception* (FoM) was calculated for different identified misconceptions (see chapter 2.2, p. 30 for more details). The FoM measure has higher validity than answers from one single item because the misconceptions are measured multiple times in different contexts and items.

Prior Knowledge: CBI pre-test

Prior knowledge was assessed as a covariate using the CBI pre-test described in more detail in chapter 2.4 and the section above. Seven items of the CBI pre-test were common with the CBI sub-test and CBI.

Cognitive Abilities

As the second covariate; *cognitive abilities* were assessed using the "Kognitiver Fähigkeitstest" (KFT) for grade 10, by Heller and Perleth (2000). The test is available for grades 4 – 12. The KFT consists of three subscales (figural, verbal, and numerical) and is based on the Berliner Intelligenzstrukturmodell (Beauducel & Kersting, 2002)). I made use of three subscales (V2, Q2, and N1, 9 minutes each) and calculated the total score of the KFT 10 as a measure of *cognitive abilities*.

Demographic Data

Additionally, the associated class, gender, and age were registered.

Procedure

I instructed and coached every teacher involved in this study on how to use the developed comparing and contrasting teaching materials before and during the time the study took place (see next section for more details). To assess students' prior knowledge, a pre-test (CBI pre-test, see chapter 2.4) was applied in the lesson before the instruction on chemical bonding started. In the following, students were taught with the comparing and contrasting teaching materials (intervention) or with conventional teaching materials, following a more sequential method of instruction (control group) for a minimum of 23 lessons. Typically the instruction took about twelve school weeks (2 lessons per week, i.e. depending on holidays about three to five months). After the instruction on all types of chemical bonding was concluded the immediate post-test (CBI subtest) was administered. I oversaw the test-taking or sent a research assistant to take the tests in the classrooms. The CBI subtest usually took about 25 to 35 minutes. Students had to finish within one lesson but were not pressured on time. Some of the participating chemistry teachers needed more than 24 lessons before they had finished with all the bonding types following their regular curriculum since they covered the intermolecular forces in more depth after the covalent bonds directly before covering ionic and metallic bonding. In this case, the test could only be applied after they had finished with all the bonding types. In all cases, the intervention group spent the same or less time on the topic than the control group. Three months after the post-test assessment was conducted, a research assistant or I applied the CBI as a follow-up test in the classrooms. Once in between the post-test and follow-up test, a research assistant or I administered the KFT 10 (assessment of cognitive abilities).

Teacher Training

To assert that the teaching materials would be implemented as intended and to compensate for the fact that the materials were totally new to the teachers, every teacher participating in my study obtained a teacher training. I provided the teaching materials and the lesson plans for each of the 23 lessons, described in chapter 4, and let the teachers go over the materials by themselves. After that I had a weekly meeting for thirty minutes to one hour on the topics that needed to be presented and how to best present the materials in class. The meetings took place in person and online. The teachers were advised not to use the material I designed in their control classes this year directly but might take over some learning activities or approaches into their materials from my input the next year when the study was completed. To control for this I collected the teachers' notes of the class (see the section on the implementation fidelity). In the interesting discussions with teachers, I also informed them about the misconceptions science students showed at the beginning of their studies at ETH Zurich. The teachers were never shown the exact questions of the CBI or the CBI pre-test.

The Comparing and Contrasting Instruction

The teaching materials are described in length in chapter 4. Hence, I only present a short description in this part. The intervention's teaching material introduces the three bonding types at the same time at the very beginning using the concept of electronegativity as the basis for distinguishing between the bonding situations. After this, the three types of bonding are explained in more detail after each other. More comparisons are prompted as soon as possible, i.e. when introducing metals after having introduced the ionic compounds in more detail. Comparing and contrasting learning activities are often used to foster awareness of the existence and differences between the three bonding types. To foster this further, an overview table is distributed and consulted during the course of the teaching unit (see chapter 4.4). The teaching unit is structured into 23 lessons. Typically teachers were able to fit the instruction into 23 lessons a few needed 24 lessons. Teachers were given some freedom how to structure their lessons. For the teaching materials to be successful the teachers were allowed to adapt the proposed sequence to address the specific classroom needs (e.g. additional time for questions if something was unclear). Larger changes were discussed beforehand in the weekly meetings.

The Conventional Instruction

The typical instruction on chemical bonds at Swiss Gymnasiums is discussed in chapter 4.1. The topics covered were the same for the intervention and the control group. The main difference lies in the sequence of instruction as well as when and how often the different bonding types are compared with each other: The conventional instruction follows a sequential order, i.e. one bonding type after each other, with a comparing lesson at the very end of the whole topic of chemical bonds and intermolecular forces. Chemistry teachers involved in my study all needed the same amount of time or more to cover the topics in their control group. This was because some teachers were discussing a few aspects in more depth in between the topics of chemical bonds (e.g. more examples of substances exhibiting intermolecular forces).

Implementation Fidelity

In a short discussion with teachers willing to participate in the study, I assessed whether the way the teachers taught about chemical bonding was too similar to the intervention method and whether the method of instruction was "conventional enough", i.e. all the important content was taught conventionally and sequentially. There was only one case where an interested teacher could not be taken into the study. The particular teacher did not introduce the bonding types simultaneously with many comparing and contrasting cases, he did, however, discuss the differentiation of the three bonding types in lengths (i.e. for several weeks) after the intervention. This setup would have resembled the intervention, hence the teacher's classes were not assessed in the study. Teachers provided me with their script of the class beforehand. I also asked for copies of students' notes to confirm that the students in the control classes were not instructed in an unconventional way, i.e. similar to the intervention. Additionally, a research assistant (on the track to becoming a teacher) or I were conducting a school visit in every class once during the study (intervention and control group) to assure that the students from the control classes were not instructed with the materials or ideas from the beforehand received comparing and contrasting teaching materials. Visits in intervention studies were conducted to assure that the provided comparing and contrasting materials were sufficiently applied and used in those classes. A protocol for every visit was made. Additionally, I stayed in contact with every participating teacher while the study took place since the teacher training was conducted over several weeks (see the section on Teacher Training above). I was asking the teachers about their experiences and questions they might have at that point and hence also controlling for the intended administration of the comparing and contrasting teaching materials.

Data Analysis

Data were analyzed with R (version 4.2.1, R Core Team, 2022) using the RStudio environment (version 2021.09.1, R Core Team, 2022). Packages used in the process were (in alphabetical order): afex (Singmann et al., 2022), data.table (Dowle & Srinivasan, 2021), effsize (Torchiano, 2020), EnvStats (Millard, 2013), eRm (Mair et al., 2021), lavaan (Rosseel, 2012), magrittr (Bache & Wickham, 2022), plyr (Wickham & Wickham, 2020), psych (Gick & Holyoak, 1983), PupillometryR (Forbes, 2020), readxl (Wickham & Bryan, 2022), semPlot (Epskamp, 2022), sjstats (Lüdecke, 2021), TAM (Robitzsch et al., 2022), tidyverse (Wickham et al., 2019).

5.4 Results

First, the comparability of the intervention and control groups, as well as the psychometric quality of the tests is described. In the following, the descriptive results are given, followed by the assessment of hypotheses 1 and 2.

Comparability and Psychometric Quality of Tests

The comparison of the intervention and control groups showed minor differences: the intervention group had a slightly higher proportion of female participants (see Table 24). Additionally, slightly lower cognitive abilities ($d = -0.27$, $CI_{95}[-0.55; 0.00]$) were detected for the intervention group using the "Kognitiver Fähigkeitstest" (KFT 10) by Heller and Perleth (2000). Since both differences are not in favor of the intervention group the differences were assessed as non-critical for the intervention study.

Table 24: Description of the Intervention and Control Group

Group	*N*	f	m	d	% f	Number of Classes	KFT, M	KFT, SD
Intervention	218	139	76	6	63.8	10	52.89	6.05
Control	108	66	40	2	61.1	5	54.45	5.02
Total	326	205	116	8	62.9	15	53.45	5.74

Note. N = number of participants, f = female, m = male, d = diverse, % f = % female, M = mean, SD = standard deviation

Internal Consistency of the Administered Tests

McDonald's omega based on polychoric correlations for ordinal scale assuming one latent factor of all tests applied to students is depicted in Table 25. The internal consistencies were good to excellent for the administered pre-test, post-test (CBI subtest), follow-up (CBI), and the KFT 10.

Table 25: McDonald's Omega Based on Polychoric Correlations for Ordinal Scale Assuming One Latent Factor of the Pre-Test, Post-Test, and Follow-Up Test as well as the KFT with its Subscales (Verbal V2, Numerical Q2, Figural N1).

				KFT (cognitive abilities, grade 10)			
ω_t of	Pre-Test	Post-Test	Follow-up	Total	Verbal	Numerical	Figural
Intervention	0.81	0.90	0.91	0.99	0.96	0.99	0.99
Control	0.81	0.91	0.90	0.99	0.95	0.99	0.99
Complete sample	0.81	0.92	0.92	0.99	0.96	0.99	0.99

Note. KFT = Kognitiver Fähigkeitstest by Heller and Perleth (2000), raw values are depicted.

Assessment of Conceptual Understanding of Chemical Bonding Models

The evaluation of students' conceptual understanding scores by time points is depicted in Table 26. At the pre-test, students in the control group started with higher means in conceptual understanding than the intervention group, however with a small effect size and mostly comparable distributions. When we assessed students' conceptual understanding at the immediate post-test the picture is reversed: students in the intervention group outperformed the control group students with a large effect size. Three months after the intervention, at the follow-up test, the difference between the two groups decreased from $M_{diff} = 4.75$ to 2.9 points, with the intervention group still outperforming the control group with a medium effect size. Regarding the seven link items that were the same across all time points, Table 27 depicts the means, standard deviations, and Cohen's *d* values with their confidence intervals. The trends are similar whereas the effect sizes are slightly lower.

Table 26: Evaluation of the Intervention's and Control Group's Conceptual Understanding of Chemical Bonding at Pre-test, Post-test, and Follow-up.

		Pre-Test Max = 23		Post-Test Max = 25		Follow-up Max = 25	
	N	M	SD	M	SD	M	SD
Intervention	218	9.52	3.92	14.4	4.64	13.6	4.83
Control	108	10.5	3.64	9.65	4.43	10.7	4.51
Cohen's *d*		-0.25		1.05		0.60	
CI_{95}		[-0.49; -0.01]		[0.78; 1.31]		[0.31; 0.89]	

Note. Max = maximum points, N = number of participants, M = mean, SD = standard deviation, CI_{95} = 95 % confidence interval, pre-test different from post-test and follow-up (7 common items)

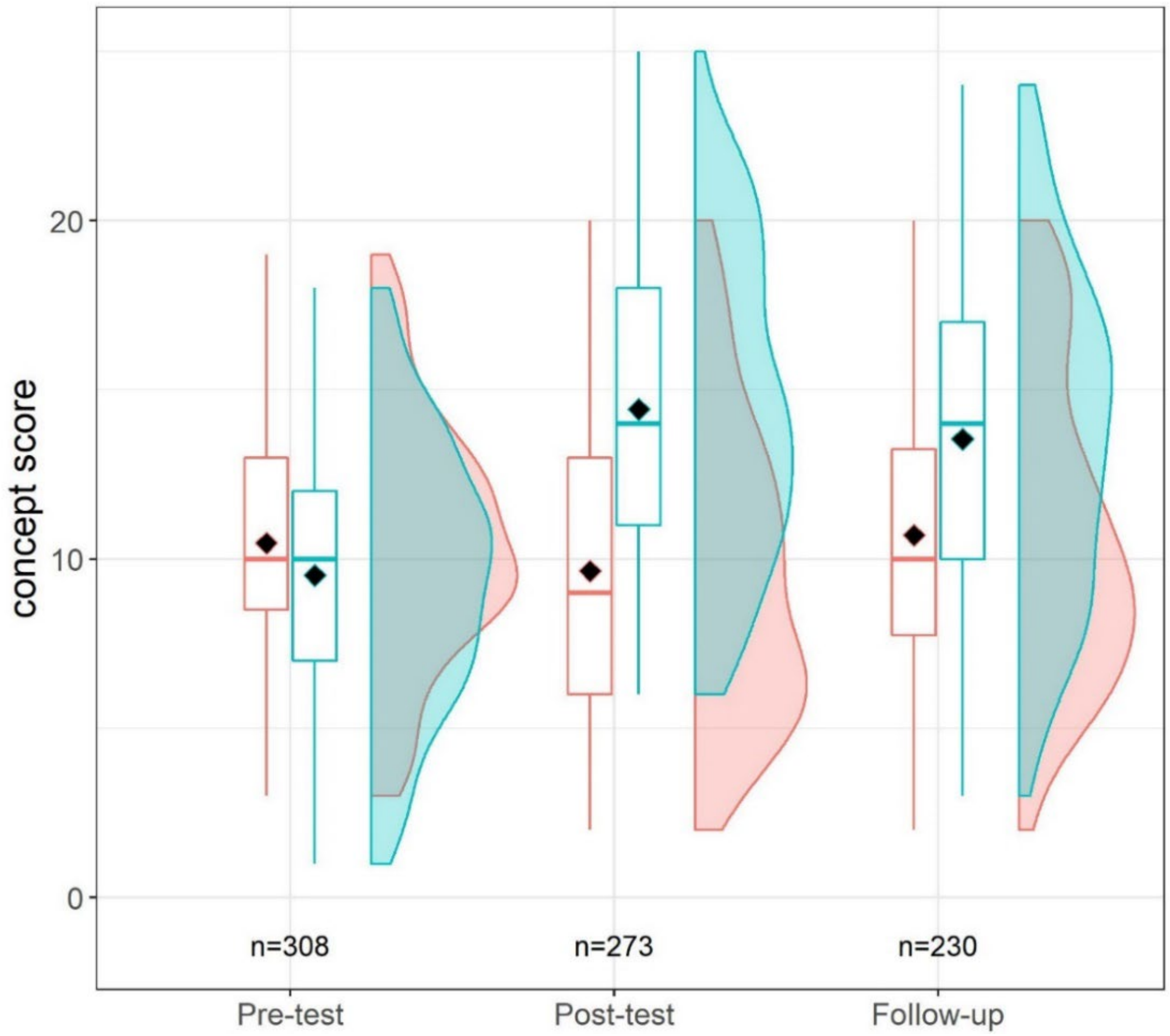


Figure 72: Conceptual understanding of the control (red) and intervention group (blue) at pre-test (max. points = 23), post-test (max. points = 25), and three months after instruction on chemical bonding (follow-up, max. points = 25), with the number of participants (n) at every time point

Table 27: Evaluation of the Intervention's and Control Group's Conceptual Understanding of Chemical Bonding at Pre-test, Post-test, and Follow-up for the seven Link Items exclusively.

		Pre-Test (Link Items) Max = 7		Post-Test (Link Items) Max = 7		Follow-up (Link Items) Max = 7	
	N	M	SD	M	SD	M	SD
Intervention	218	1.87	1.04	4.45	1.56	4.25	1.60
Control	108	2.17	0.98	3.58	1.51	3.71	1.61
Cohen's *d*		-0.29		0.56		0.34	
CI_{95}		[-0.54; -0.06]		[0.30; 0.82]		[0.06; 0.62]	

Note. Max = maximum points, N = number of participants, M = mean, SD = standard deviation, CI_{95} = 95 % confidence interval

Hypothesis 1: Effect of Comparing and Contrasting on Conceptual Understanding

Does comparing and contrasting teaching material foster conceptual understanding more strongly than conventional teaching methods? I hypothesized that the intervention students will outperform the control group students in terms of conceptual understanding (1) at the post-test as well as (2) at the follow-up test. Since this study took place in regular classes, no random assignment within the class was possible. Hence, I also assessed students' *cognitive abilities* and *prior knowledge* as covariates. How do those factors influence learning in this study? To control for those effects, I ran a multilevel model on the post-test as well as the follow-up test score predicted by *prior knowledge* (pre-test score), *experimental group* (intervention or control), and *cognitive ability* (KFT 10 total). Additionally, I ran a repeated measurement analysis of covariance (rmANCOVA) with the seven link items that were present in all three tests (pre-test, post-test, and follow-up test) while controlling for *cognitive abilities* (KFT 10 total).

Multi-level Analysis for the Prediction of Post-Test Scores

To control for the dependency of the students in their classes, I modeled the data as nested in classes as a random intercept model. The Intra-Class-Correlation was at 29.2, indicating large variability between the classes. Table 28 shows the results of the multilevel model. There was a main effect of *prior knowledge:* students who scored 1 point above average in the pre-test scored 0.57 points more in the post-test. There was a main effect of *group* associated with the intervention group scoring 5.37 points more than the control group on average. There was neither a significant effect of *cognitive ability* nor any significant interactions. The model suggests that the intervention influences the post-test score strongly when cognitive abilities and prior knowledge are considered as factors. Hence providing strong support in favor of hypothesis 1 at post-test.

Table 28: Parameters of the Linear Mixed Model for the Prediction of Post-Test Scores while Controlling for Prior-Knowledge, Cognitive Abilities, and Students Being Nested in Classes.

	Estimate	SD	*df*	*t*	*p*
(Intercept)	9.26	1.09	12.26	8.522	< .001 ***
Prior knowledge (pre-test score)	0.57	0.13	181.63	4.49	< .001 ***
Cognitive Ability (KFT 10 total)	0.11	0.09	178.72	1.182	.23
Group (intervention or control)	5.37	1.35	11.99	3.988	< .01 **
Prior knowledge : Cognitive abilities	0.04	0.02	184.41	1.47	.14
Prior knowledge : Group	0.18	0.16	187.72	1.13	.26
Cognitive abilities : Group	0.05	0.11	179.49	0.51	.61
Prior knowledge : Cognitive abilities : Group	-0.04	0.03	184.12	-1.314	.19

Note. SD = standard deviation, *df* = degrees of freedom

Multi-level Analysis for the Prediction of Follow-up-Test Scores

Applying the same model for the follow-up test scores yielded comparable results: Again, there was a main effect of *prior knowledge:* students who scored 1 point above average in the pre-test scored 0.49 points more in the follow-up test (see Table 26, p. 148 for means and standard deviations). A marginally significant effect (p = .076) of *group* was detected with the intervention group scoring 2.51 points more than the control group on average. Again, there was no significant effect of *cognitive ability* and no significant interactions. Given, that the number of participants was lowered at follow-up (230 compared to 273 at post-test) due to two classes being on a language exchange, the lowering of power was to be expected. However, Cohen's d of 0.60 and its 95% confidence intervals ([0.31; 0.89]) for the difference in follow-up conceptual understanding scores strongly point to a relevant effect. Those results support hypothesis 1 at follow-up at the significance level of $p < .1$.

Table 29: Parameters of the Linear Mixed Model for the Prediction of Follow-up-Test Scores while Controlling for Prior-Knowledge, Cognitive Abilities, and Students Being Nested in Classes.

	Estimate	SD	*df*	*t*	*p*
(Intercept)	10.86	1.02	8.61	10.61	< .001 ***
Prior knowledge (pre-test score)	0.49	0.16	149.33	3.15	.002 **
Cognitive Ability (KFT 10 total)	0.10	0.12	150.49	0.82	.41
Group (intervention or control)	2.51	1.24	8.37	2.03	.08
Prior knowledge : Cognitive abilities	0.01	0.03	158.90	0.24	.81
Prior knowledge : Group	0.19	0.20	157.82	0.96	.34
Cognitive abilities : Group	0.01	0.13	151.73	0.10	.92
Prior knowledge : Cognitive abilities : Group	-0.01	0.03	158.55	-0.23	.82

Note. SD = standard deviation, *df* = degrees of freedom

Repeated-Measures Analysis of Covariance for Link Items

A repeated measures analysis of covariance (rmANCOVA) was conducted using a score of 7 link items over three time points (pre-test, post-test, and follow-up test) with *cognitive abilities* as a covariate. The results reveal an effect of *group* ($F(1, 156) = 10.47, p = .001, \eta_G^2 = .04$), *cognitive abilities* ($F(1.94, 303.07) = 13.69, p < .001, \eta_G^2 = .05$), and *time* ($F(1.94, 303.07) = 27.41, p < .001, \eta_G^2 = .08$). There was a significant interaction between time and group ($F(1.94, 303.07) = 12.50, p < .001, \eta_G^2 = .04$). This supports the hypothesis that students' understanding changes over time when only assessing link items across all three time points. The significant effect of *group* is again in line with the intervention improving conceptual change more strongly than the control group.

Table 30: Results of the Repeated Measures ANCOVA Regarding Link Items of the Conceptual Understanding Inventory

Effect	*df*	*MSE*	*F*	η_G^2	*p*
Group (intervention or control)	1, 156	3	10.47	0.04	.001 **
Prior knowledge (pre-test score)	1, 156	3	13.69	0.05	< .001 ***
Time	1.94, 303.07	1.33	27.41	0.08	< .001 ***
Group : Time	1.94, 303.07	1.33	12.5	0.04	< .001 ***
Prior Knowledge : Time	1.94, 303.07	1.33	2.06	0.01	.13

Note. df = degrees of freedom, MSE = Mean Squared Error, η_G^2 = generalized eta-squared

Overall, the used models support hypothesis 1, that comparing and contrasting activities are the reason for the higher gains in conceptual understanding. The effect was more pronounced at the post-test than three months after the intervention (at the follow-up test). This is due to two reasons: (1) students in the intervention group decreased significantly but with a negligible effect size in their conceptual understanding scores over the course of three months (paired *t*-test: $t(148) = 2.26, p = .025; d = -0.19$, $CI_{95}[-0.40; 0.03]$) and (2) students in the control group increased their scores over the same period of time with a small effect size (paired *t*-test: $t(67) = 3.21, p = .002; d = 0.24$, $CI_{95}[-0.08; 0.55]$). Since the concepts of the different bonding situations were used on regular basis also after the topic has been covered explicitly, students in the control group might have used the opportunities to better incorporate the concepts into their mental network. Students in the control group started with relatively low post-test scores, wherefore one might hence argue with an effect of the regression to the mean. In contrast to that, the intervention's students were at relatively high levels of conceptual understanding and were hence more prone to decrease their scores.

Hypothesis 2: Effects of the Intervention on the Prevalence of Misconceptions

Assessing the prevalence of misconceptions three months after the intervention yields a mean score and standard deviation for each of the identified misconceptions. From this, *frequencies of misconceptions* (FoM) are calculated by dividing by the maximum points for a specific misconception. The FoM values for the intervention and control group, the corresponding Cohen's *d* values, and confidence intervals for the differences between FoM values are depicted in Table 31.

Table 31: Comparison of Frequency of Misconceptions of the Intervention and Control Group at Follow-up

		Intervention			Control			Cohen's *d*	
Misconception	Max points	M	SD	FoM	M	SD	FoM	*d*	CI_{95}
Overgeneralization	21	4.5	2.97	0.22	6.67	3.68	0.32	0.66	**0.38; 0.95**
NaCl molecule	11	1.77	1.69	0.16	2.83	2.24	0.26	0.57	**0.28; 0.85**
Subunit or pairs in salts	6	1.00	1.11	0.17	1.20	1.10	0.20	0.24	-0.04; 0.52
IMF in metals	3	0.84	1.02	0.28	1.31	1.17	0.44	0.43	**0.15; 0.72**
IMF in ionic compounds	2	0.44	0.69	0.22	0.72	0.79	0.36	0.39	**0.11; 0.68**
IMF within molecules	4	1.75	0.99	0.44	1.74	1.05	0.44	-0.01	-0.29; 0.27
Ionic lattice	1	0.34	0.47	0.34	0.79	0.41	0.79	1.00	**0.71; 1.30**
Metallic lattice	4	0.81	1.24	0.20	2.08	1.26	0.52	1.02	**0.72; 1.31**

Note. M = mean, SD = standard Deviation, FoM = frequency of misconception, IMF = intermolecular force, *d* = Cohen's *d* for the FoM values, CI_{95} = 95 % confidence interval. Bolded values show cases in which the groups differed significantly.

I hypothesized that the intervention group's students were exhibiting lower frequencies of misconception three months after the instruction of the topic. To assess if this holds, the frequencies of misconceptions were hence assessed three months after the intervention. With the exception of the *intermolecular forces within a molecule* and the *subunit or pairs in salts* misconceptions, the intervention group was exhibiting fewer signs of the prevalence of misconceptions. The effect sizes of the differences in the frequencies of misconceptions range from *d* = 0.24 (existence of *subunit or pairs in salts*) to 1.02 (misconceptions concerning *metallic lattices*). Hypothesis 2 is hence strongly supported by the findings of this study.

Analyzing Conceptual Change with Sankey Plots

Item Q6 of the CBI (see Figure 14, p. 45) is one of the link items present in all three tests. Analyzing the proportion of misconceptions at this item by timepoint can potentially give an insight into the state of students' mental representation of sodium chloride at pre-test, post-test, and follow-up. When asked how sodium chloride is represented in this compound students chose between different mental representations. Students can choose between the correct representation of sodium chloride (Correct in Figure 73 and Figure 74), synthetic models (Synth2 and Synth1) as well as covalent models (Covalent2 and Covalent1).

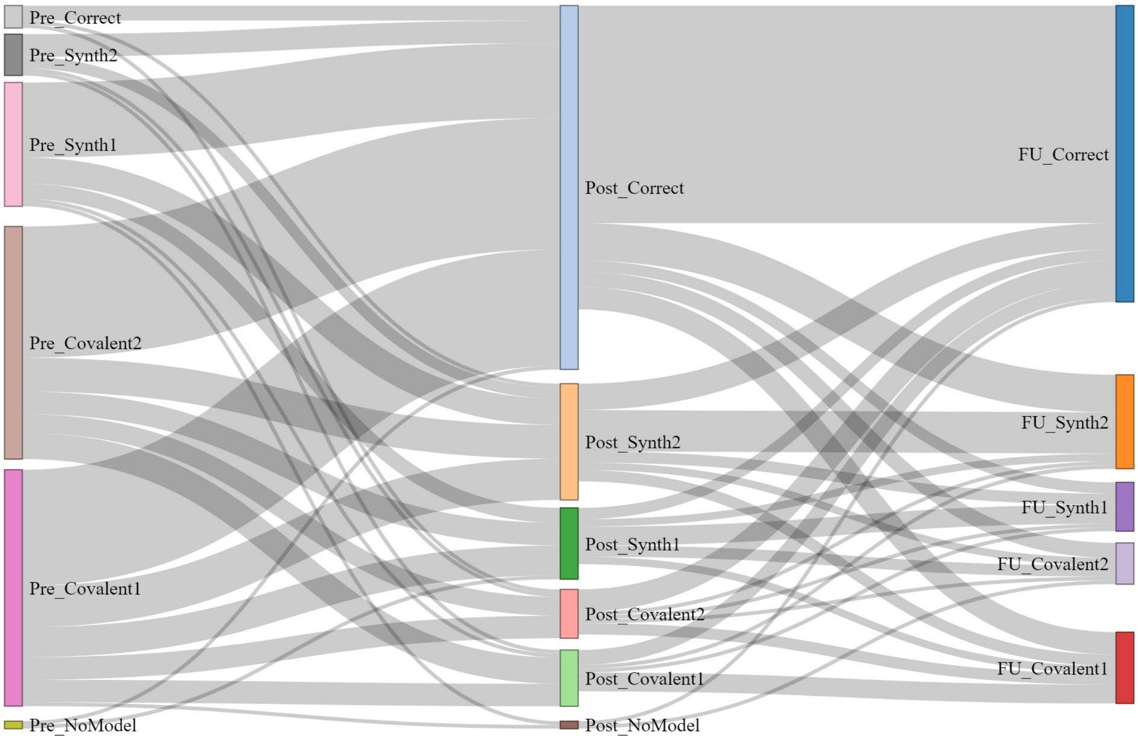


Figure 73: Sankey plot of item Q6 for the distribution of mental representations of the intervention group's students at pre-test (left), at post-test (middle), and follow-up (right). From top to bottom; correct to least scientifically correct concept: Correct = accurate model of sodium chloride, Synth2 = synthetic model 2 (subunit representation), Synth1 = synthetic model 1 (ions but represented as molecules), Covalent2 = Sodium chloride as molecules made of neutral atoms, Covalent1 = neutral atoms in a lattice structure, NoModel = no model chosen.

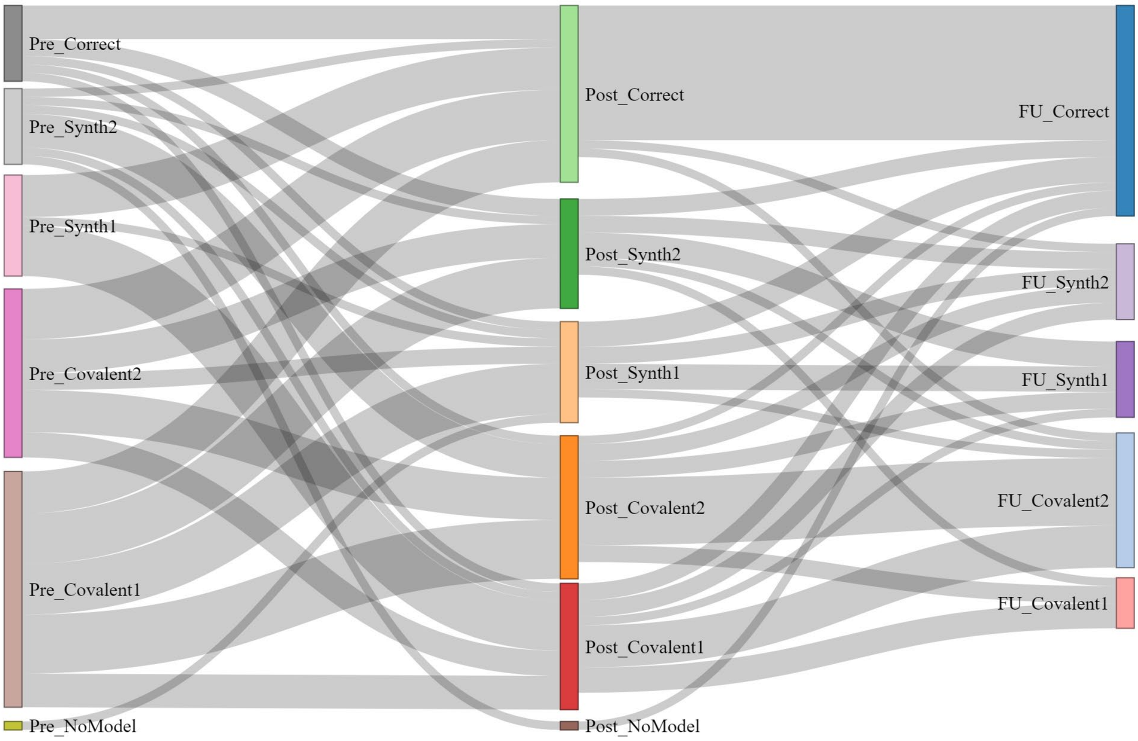


Figure 74: Sankey plot of item Q6 for the distribution of mental representations of the control group's students at pre-test (left), at post-test (middle), and follow-up (right). From top to bottom; correct to least scientifically correct concept: Correct = accurate model of sodium chloride, Synth2 = synthetic model 2 (subunit representation), Synth1 = synthetic model 1 (ions but represented as molecules), Covalent2 = Sodium chloride as molecules made of neutral atoms, Covalent1 = neutral atoms in a lattice structure, NoModel = no model chosen.

The Sankey plots are ordered such that the more scientifically correct model is on top. It can be observed that at pre-test (left column) the control group (Figure 74) had higher percentages of students leaning towards the more scientifically correct models (Correct, Synth2 and Synth1) as the intervention group (Figure 73). At the post-test (middle column) the differences between the two groups were most salient: Whereas in the intervention group the majority of students chose the correct model or synthetic models, about 40 % still held a mental representation of a covalent bonding situation (Covalent2 and Covalent1). At the follow-up test (right column) the reduction in the number of participants was noticeable, rendering the interpretation more challenging. Overall we can observe the general trend that the students in the intervention group were slightly decreasing (about 5 % when controlling for lower student numbers) their number of students holding a correct model, whereas the control group's students increase their number of more correct representations (about 20 % gain in Correct). Still, when comparing the intervention to the control group, the shares of students holding the correct and synthetic models are higher for the intervention group. This finding also supports the more generalizable results from the frequency of misconception measure.

5.5 Discussion

Does the new teaching material foster conceptual understanding of chemical bonding more strongly than conventional instruction? The answer to this question is a clear *yes*. Despite lower cognitive abilities, lower prior knowledge, same or less amount of time spent on the topic, students in the intervention group profited more from the instruction on chemical bonds than the control group. The intervention group outperformed the control group in the post-test and follow-up test. Additionally, they held significantly fewer misconceptions three months after the intervention. The medium to large effect sizes I reported and the multi-level models controlling for *prior knowledge*, *cognitive abilities,* and *nesting in classes* support the hypothesis that the main reason for the differences in conceptual understanding lies in the intervention.

The implementation of more comparing and contrasting activities and the simultaneous introduction of all bonding types clearly supports students in increasing their awareness of the existence and differences between the three bonding types. Furthermore, the conceptual understanding was acquired in a sustainable manner, evaluated by the slightly decreased but still high levels of conceptual understanding three months after the intervention.

6 Evaluation of the Condensed Teaching Materials for a University Preparatory Course

The *university evaluation studies 1 – 2* revealed that students planning to study chemistry or biochemistry lack fundamental conceptual understanding concerning chemical bonding. Despite being previously instructed on the topic, high frequencies of misconceptions were detected in very selective student samples (see chapter 2 for details). What can be done to change this? One possibility is to adjust the way we teach on the Gymnasium level: With the developed teaching materials I presented a viable option that has been successfully applied and evaluated (see chapter 4 for the teaching materials, chapter 5 for evaluation in upper secondary school). Another possibility is to influence students' conceptual understanding after they have been previously instructed on the topic. Shtulman and Valcarcel (2012) have shown with their speed-reasoning tasks that naïve theories coexist even in experts' mental representations (indicated by the response time difference between consistent and inconsistent statements). However, experts show higher accuracies than novices even under time pressure. From this it follows that (1) it is possible to improve in accuracy despite the previously described prevalence of naïve theories and intuitions and (2) when we want to learn about conceptual change, it can help to take a closer look at the difference between novices and experts. Experts have found ways how to suppress naïve theories or misconceptions more efficiently by acquiring more scientifically sound concepts to counter-intuitive ideas. To formulate this more positively, it is hence possible to add to preexisting concepts or naïve theories. The question remains, how such a process of acquisition of a novel concept is facilitated most efficiently. The developed teaching materials (23 lessons) have proven to tackle many preexisting naïve theories or misconceptions in the making (see chapter 4 for concrete examples of how this is done). I hence used the teaching materials as a basis for the design of a preparatory course for science students before they started their studies at ETH Zurich. Students were not new to the topic and I hence planned to compress the teaching unit such that it would fit into 7 lessons. The main research questions for this study were:

1. Is it possible to foster newly enrolled university students' conceptual understanding of chemical bonding with a short preparatory course before attending lectures?

2. Can the frequency of misconception substantially be lowered with a preparatory course of seven lessons?

6.1 Brief Overview of the Study Design and Hypotheses

The *university intervention study* was set up as a pre-post-test intervention study applying the previously described *Chemical Bonding Inventory* (CBI, see chapter 2 for more details) up to four times. The CBI assesses students' (1) *conceptual understanding* as well as (2) the *prevalence of misconceptions* (with the frequency of misconception measure). After an online pre-test, half of the students took a retest at the beginning of the preparatory course to assess whether there was a learning effect by test-taking. In seven lessons, I then instructed the students with comparing and contrasting teaching materials developed for the Gymnasium level but in a more compressed version. The CBI was administered immediately after the course (post-test) as well as one to two weeks after the instruction (follow-up test). The study design is illustrated in Figure 75.

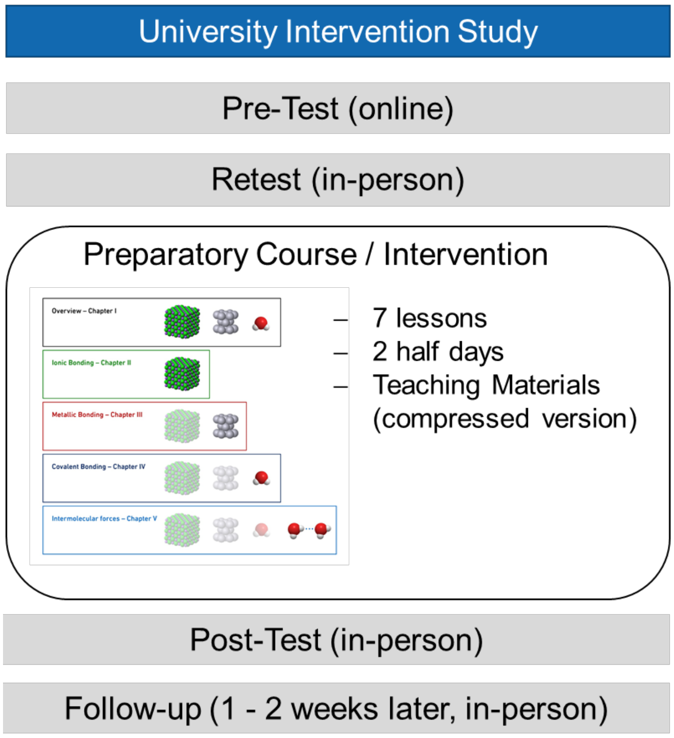


Figure 75: Design of university intervention study, with four assessments of conceptual understanding (pre-test, retest, post-test, and follow-up).

Hypotheses

Acknowledging the coexisting nature of naïve and scientific concepts, it is possible to add to conceptual understanding regardless of the level of understanding of a topic. Hence the preparatory course should benefit students' conceptual understanding. The difference to the Gymnasium intervention studies lies in the fact that students are instructed in a very fast and condensed format (approximately one-third of the time as normal teaching). Due to the strict time constraints, there was less time available for students to go through all the thought processes designed to promote conceptual change. Students had less time to actively construct their knowledge themselves and make important inferences on their own (e.g. Förtsch et al., 2017; Lombardi et al., 2021). This is counteracted by the fact that they have already been instructed on the topic and that the sample attending courses is more selective than "regular" school classes. Regarding the reduction of misconceptions: Whereas students have already been instructed and potentially influenced by previous teaching and overgeneralization it is still possible to give students appropriate means of how to counter those naïve concepts or theories. Hence, I formulated the following hypotheses:

Hypothesis 1: Students taking part in the preparatory course improve their conceptual understanding from pre-test to post-test beyond test-taking effects.

Hypothesis 2: The frequencies of misconceptions is reduced from pre- to post-test.

Whether the potential learning gains are sustainable will be evaluated in this study, using the follow-up test.

6.2 Methods

Sample

The student recruitment. One week before the semester start in the fall of 2021, I was allowed to write an email to the students that would make up the *university evaluation sample 2* (see chapter 2 for more details on the sample). Students participating in this study, i.e. the u*niversity intervention sample*, are hence a sub-sample of the *university evaluation sample 2* (with a few exceptions for students not taking part in the follow-up intervention). Participation was voluntary, but the interest in the course was high. Due to restrictions regarding the Covid-19 pandemic, not all students were able to participate: New guidelines were implemented a few days before the intervention started. Still, a total of 293 students participated in the preparatory course (approximately 30 % of all the invited students). Students had the opportunity to consent to the data usage or not. The data was collected anonymously with a student-generated code (see the first page of tests, e.g. appendix 1.1) in accordance with the ETH Zurich Ethics Commission (see appendix 2, EK-2021-N-123). Students were not compensated for their participation in the study.

The ***University intervention sample*** consisted of 293 newly enrolled, first-year science students (67.9 % female, mean age of 19.6 years (SD = 1.6). Students reported an average of 3.6 years of prior chemistry education and 46 % of the students had chosen chemistry as a special subject (i.e. extra classes with a focus on chemistry). The interest in four different subjects was assessed on a scale from 1 (very low) to 5 (very high): 4.2 for chemistry, 4.2 for biology, 3.7 for physics, and 3.5 for mathematics. The number of participants per study subject in the *university intervention study* (this study) and *university evaluation study 2* (described in chapter 2) is depicted in Table 32 for comparison.

Table 32: Comparison of Students per Study Subject in the University Evaluation Sample 2 and University Intervention Sample (this study)

	University Evaluation Sample 2 (2021)	*University Intervention Sample (Taking Part in the Preparatory Course)*
Field of study	*N*	*N*
Agricultural Sciences	33	13
Biochemistry	58	15
Biology	93	38
Chemical Engineering	31	8
Chemistry	62	18
Earth and Climate Sciences	44	14
Environmental Engineering	57	17
Environmental Sciences	134	33
Food Sciences	69	23
Health Sciences and Technology	233	57
Interdisciplinary Sciences	52	20
Pharmaceutical Sciences	104	37
	970	**293**

Measures

Conceptual Understanding of Chemical Bonding Models

The conceptual understanding was assessed using the developed *Chemical Bonding Inventory* (CBI, see chapter 2 for more details). The CBI was administrated as an online test three to four times: shortly before the start of the preparatory course (online at home), directly before the start of the instruction for half the sample (retest, in-person), immediately after (post-test, in-person) and 1 to 2 weeks later in the first tutoring lessons (follow-up, in-person). The CBI allows for the calculation of a *total score* as well as five subscores of conceptual understanding. There is a subscore for each bonding type (*Ionic*, *Metallic,* and *Covalent*), a subscore for the understanding of intermolecular forces (*IMF*) as well as a subscore describing the formal identification of a bonding situation from the chemical formula (*Identification*).

Frequency of Misconceptions

As described in more detail in chapter 2, a measure for the evaluation of the prevalence of misconceptions was used: the *frequency of misconceptions* (FoM) (see p. 26 for an example). Single incorrect answers pointing towards the prevalence of a certain misconception were counted and added up for all items of the CBI resulting in a mean score for every misconception. Dividing by the total number of distractors taping into this misconception, a *frequency of misconception* (FoM) was calculated for different identified misconceptions (see chapter 2.2, p. 30 for more details). The FoM measure has higher validity than answers from one single item because the misconceptions are measured multiple times in different contexts and items.

Demographic Variables and Motivation

Students' age, gender, and motivation for chemistry, biology, physics, and mathematics were assessed with an online questionnaire before the start of the preparatory course. Students additionally self-reported their *prior chemistry education* (years of chemistry) and whether they had chosen a *special focus in chemistry* in upper secondary school. Additionally, the field of future study at ETH Zurich was registered.

Procedure

To assess (1) the change in conceptual understanding and (2) the level of prevalence of misconceptions the CBI was administered up to four times. Students were asked to fill out the online pre-test questionnaire 2 – 5 days before the start of the preparatory course. A few questions inquiring about their demographic variables, prior chemistry education, and interest in science were added in front of the CBI (see measures section). The online-based questionnaire software of *Qualtrics International Inc.* was used for the CBI.

The preparatory course took place in a lecture hall at ETH Zurich with 338 seats. At the time there were still regulations in place due to which only half of the room was allowed to be filled. Hence I split the 293 students into two groups of approximately 150 students. The instructions of the two groups were the same. The preparatory course took place on two half days with four hours being present. One group was taught from 8 – 12 am, whereas the other was taught in the afternoon from 1-5 pm on Thursday and Friday in the week before the start of the fall semester 2021. At the beginning of the course, I asked half of the lecture hall to retake the test (evaluation of retest effect). The evaluation was conducted in person with my supervision but on every student's own laptop. The other half was given some web links to inform themselves about extracurricular activities at the university and asked to come back 30 minutes later. I then instructed the students on two half days (four hours per day). In the last of the eight lessons, students were asked to fill out the post-test. The follow-up assessment was conducted in the first tutoring classes, one to two weeks after the intervention. Students were again asked to fill out the CBI on their laptops with no auxiliaries and under the supervision of a tutor. The difference between students stems from the fact that the tutoring lessons were set up at different times depending on the study subject and tutoring groups the students were assigned to.

Teaching Materials and Instruction

I used the teaching materials described in chapters 4.3 and onwards as the basis to instruct the students. How did the instruction in this preparatory course differ from the instruction at the Gymnasium level? First the general differences are given, then the changes made to the teaching unit are described in more detail (i.e. which worksheets have been left out due to time restraints) before describing what has been added compared to the teaching materials prepared for the Gymnasium.

General Differences

The general differences can be summed up as follows:

- Instruction in 7 lessons (of approx. 50 minutes) instead of 23 lessons (of 45 minutes)
- An increased pace of instruction
- More direct instruction
- Less time for worksheets and discussions of worksheets
- Some worksheets were not discussed in class or were completely left out (see the following paragraph)

Excluded Teaching Materials

Due to time restraints some worksheets were not discussed in class but distributed (indicated with an asterisk (*) in the list below). Worksheets that were not even distributed were colored in red. The time invested for each chapter was reduced significantly for this preparatory course (given in brackets in the title of the following list).

Chapter 1: Overview (1 lesson)

- Added a 5-minute repetition on Coulomb's law in front of the teaching unit

Chapter 2: Ionic Bonding (2 lessons)

- Worksheet II/2, tasks 2 and 3 (*)
- Worksheet II/4, task 2 (*)
- Worksheet II/5, task 1 (*)
- Nomenclature of salts (*)
- Concept Map (*)

Chapter 3: Metallic Bonding (1 lesson)

- Worksheet III/2 (*)
- Worksheet III/3 (not distributed)

Chapter 4: Covalent Bonding (2.5 lessons)

- Worksheet IV/4 (not distributed)

- Worksheet IV/5: Drawing of Lewis structures was assumed to be understood (not distributed)
- Worksheet IV/6, tasks 2 and 3 (*)
- Worksheet IV/7 (*)
- Worksheet IV/9: VSEPR-model was only introduced, but not trained during the course
- Concept Map (not distributed)

Chapter 5: Intermolecular Forces (0.5 lessons)

- Worksheet V/2 (not distributed)
- Worksheet V/3 (not distributed)
- Worksheet V/4, task 1, task 3 (*)
- Worksheet V/5 (only short introduction on page 1)

Note: Students were given the solutions to all the worksheets for self-study after the course. Students had in theory time to look at the solutions of the exercises not discussed in class (but distributed). The post-test was conducted in the last lesson of day 2, i.e. students only had time to review solutions for chapters 1 – 2 before filling out the post-test.

Addition to the Teaching Materials

Before the instruction on the bonding types started, I added a repetition section on Coulomb's law. I also added a short review of the most prominent misconceptions and a scientifically more accurate description after chapters 1, 2, and 3 to foster students' awareness of those difficulties. Those were some keywords on the wrong concepts (in red) and the more accurate conception in green. This differs from the original teaching unit: Misconceptions are also actively countered with means of self-explanation tasks taking up common misconceptions or by comparison of different models incorporating misconceptions (see worksheet II/4 in appendix 3, for an example). However, the misconceptions are neither discussed explicitly nor named and listed as such. Since students had less time to solve the exercises, especially targeting and taking up such misconceptions this was deemed an efficient way to revisit the misconceptions. The questions of the questionnaire were of course not discussed during the preparatory course.

Data Analysis

Data were analyzed with R (version 4.2.1, R Core Team, 2022) using the RStudio environment (version 2021.09.1, R Core Team, 2022). Packages used in the process were (in alphabetical order): afex (Singmann et al., 2022), data.table (Dowle & Srinivasan, 2021), effsize (Torchiano, 2020), EnvStats (Millard, 2013), eRm (Mair et al., 2021), lavaan (Rosseel, 2012), magrittr (Bache & Wickham, 2022), plyr (Wickham & Wickham, 2020), psych (Gick & Holyoak, 1983), PupillometryR (Forbes, 2020), readxl (Wickham & Bryan, 2022), semPlot (Epskamp, 2022), sjstats (Lüdecke, 2021), TAM (Robitzsch et al., 2022), tidyverse (Wickham et al., 2019).

6.3 Results

Descriptive Statistics

The students' conceptual understanding total scores of the CBI and their distribution at different time points are depicted in Table 33 and Figure 72. McDonald's omega based on polychoric correlations for ordinal scale assuming one latent factor for the administered CBI is given in the last row of Table 33. The internal consistencies of the CBI were excellent at all four measurement time points.

Table 33: Conceptual Understanding Total Scores and McDonald's Omega of the CBI at Four Time Points.

	Pre-Test	Retest	Post-Test	Follow-Up
N	280	141	253	223
Max	31	31	31	31
M	9.87	9.84	22.2	20.7
SD	5.05	5.60	5.06	5.20
ω_t	.92	.94	.93	.92

Note. N = number of participants, Max = maximum points, M = mean, SD = standard deviation, ω_t = McDonald's omega based on polychoric correlations for ordinal scale assuming one latent factor

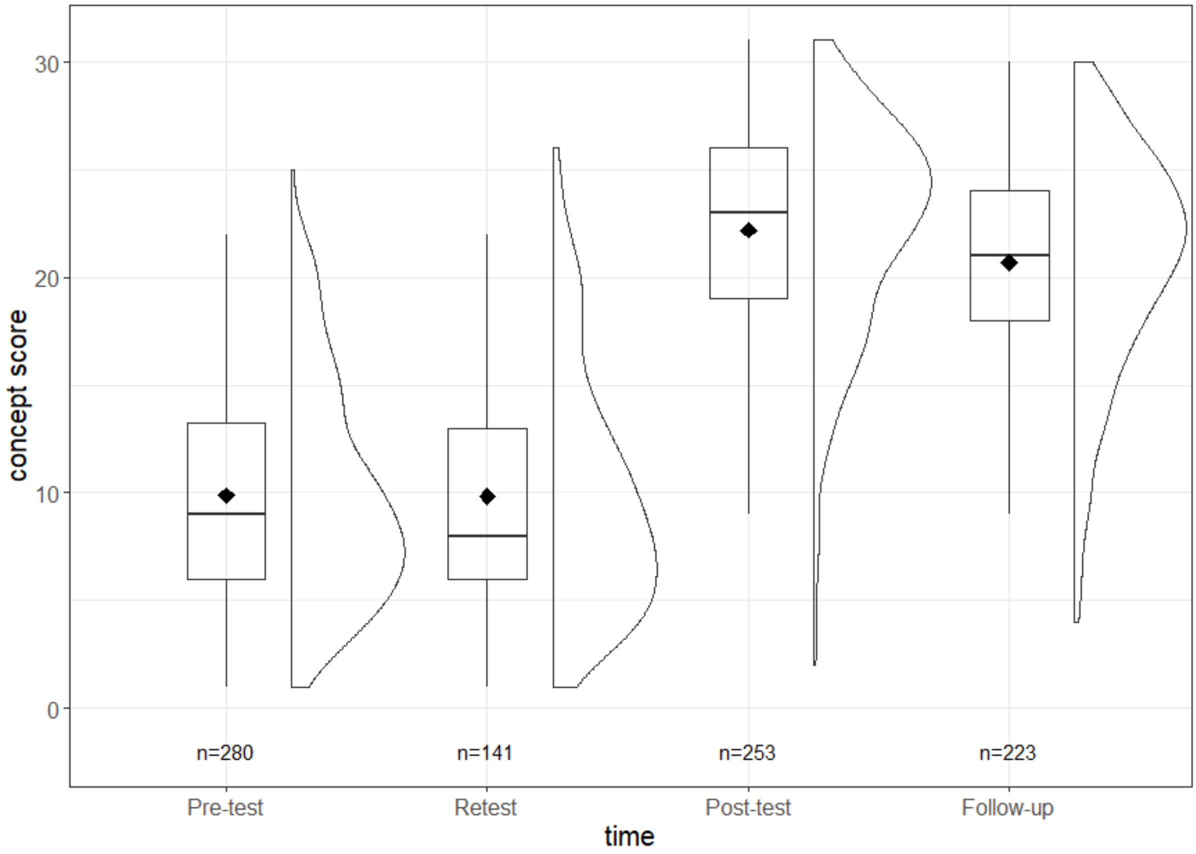


Figure 76: Conceptual understanding total score of the CBI at pre-test, retest, post-test, and follow-up test (max. points = 31), with the number of participants (n) at every time point.

Assessing Test-Retest Reliability

To rule out a possible retest effect, I evaluated the test-retest reliability with half of the sample (N = 141). The test-retest reliability was determined at *r*(136) = .89, *p* < .001. Students did not improve their scores by simply trying to solve the test twice (see Table 33, p. 163 for means and standard deviations). Students taking both tests, a small but insignificant decrease by 0.031 points on average is detected (paired t-test; *t*(135) = -1.42, *p* = .16) associated with a negligible effect size (*d* = -0.007, CI_{95}[-0.21; 0.20]). To conclude: A strong increase in conceptual understanding due to retaking the test has not been observed, and the test-retest reliability is high.

Effect of the Preparatory Course on Conceptual Understanding

To answer research question 1, whether the preparatory course fosters the conceptual understanding of chemical bonding, I first ran a repeated measures analysis of variance (rmANOVA) across pre-test, retest, post-test, and follow-up. I then investigated the changes in conceptual understanding from pre-test to post-test and from post-test to follow-up regarding their (1) *total score* and (2) their *subscores.* I hypothesized that the students will increase their conceptual understanding scores from the pre-test to post-test (hypothesis 1).

The repeated measures analysis of variance (rmANOVA) across pre-test, retest, post-test, and follow-up test supports the hypothesis for a change of conceptual understanding in regards to the total score: I report a strong effect of time (*F*(1.84, 196.59) = 637.77, *p* < .001, $\eta_G^2 = .60$).

Assessing Pre-Test to Post-Test Increase in Conceptual Understanding

Students increase their understanding in a very substantial manner: Starting at 9.87 points out of 31 points, students score 22.2 points on average in the post-test (see Table 33, p. 163). A large and significant effect is detected (paired t-test; *t*(246) = 41.5, *p* < .001; Cohen's *d* = 2.44, CI_{95}[2.21; 2.66]). These findings support hypothesis 1: the conceptual understanding is increased from the pre-test to the post-test.

Assessing the Sustainability of the Increase in Conceptual Understanding

Is the increase in conceptual understanding sustainable? Assessing students one to two weeks after the intervention reveals: Students still score high (M = 20.7, SD = 5.2) but significantly lower than in the post-test (paired t-test; *t*(206) = -5.49, *p* < .001). Students taking both tests score 1.14 points lower on average associated with a small effect size (*d* = 0.30, CI_{95}[0.12; 0.48]).

Assessing Conceptual Understanding Subscores of the CBI

I detected a high rise of conceptual understanding from pre- to post-test and a small decrease at follow-up. Are the increase and decrease homogenous across all sub-domains? An analysis of the CBI's conceptual subscores reveals that students improve across all bonding types from pre-test to post-test (see Table 34). On the other hand: Students' understanding decreased at the follow-up (1 – 2 weeks after the preparatory course). Finding out where exactly a decrease in conceptual understanding is occurring after this short period of time is at least as interesting as seeing the strong increase of conceptual understanding from pre- to post-test: It can direct our attention to where sustainable conceptual change is a harder feat. The analysis of the subscores' solution rates yields answers to this question: The subscores for the *ionic* and *metallic* bonding as well as the *identification* subscore are stable from post-test to follow-up. However, the subscores of *covalent bonding* and *intermolecular forces* seem not to be as stable (highlighted in red in Table 34).

Table 34: Students' Total and Subscores for Conceptual Understanding of Chemical Bonds at Pre- and Post-Test

		Pre-Test			Post-Test			Follow-up		
	Max points	M	SD	SR	M	SD	SR	M	SD	SR
Total Score	31	9.87	5.05	.32	22.2	5.06	.72	20.7	5.2	.67
Ionic	12	4.08	1.9	.34	8.55	1.56	.71	8.29	1.69	.69
Metallic	8	2.62	1.67	.33	6.21	1.47	.78	6.14	1.51	.77
Covalent	8	2.71	1.63	.34	**5.37**	1.79	.67	**4.82**	1.74	.60
IMF	8	2.06	1.5	.26	**4.55**	1.66	.57	**3.83**	1.68	.48
Identification	7	3.81	1.96	.54	5.97	1.44	.85	5.96	1.36	.85

Note. M = mean, SD = standard deviation, SR = solution rate. Subscores with a decrease from the post-test to the follow-up test are highlighted in red.

Compared to the post-test, students performed 0.55 points lower on average in the follow-up score of *covalent bonding* (paired t-test; $t(206) = 4.44$, $p < .001$, $d = 0.31$, $CI_{95}[0.13; 0.49]$) and 0.72 points lower in the *intermolecular forces score* (paired *t*-test; $t(206) = 5.88$, $p < .001$, $d = 0.43$, $CI_{95}[0.24; 0.61]$). Both effect sizes in the decrease of conceptual understanding of covalent bonds as well as intermolecular forces are significant but small. *Intermolecular forces* were only discussed for approximately 30 minutes despite being a complicated topic – explaining the decrease after this short period. More interestingly, the *covalent bonding* subscore decreases despite being instructed for the longest period of time (2.5 of 7 total lessons). After this initial finding, I analyzed the items with the biggest decrease and came to the conclusion that all items tested for an overgeneralization of the covalent bond: e.g. molecule definition (Q3 of CBI, see appendix 1.1) or where intermolecular forces occur (Q17 of CBI, see appendix 1.1). This finding is in line with the identification of the biggest challenge for understanding chemical bonding; the tendency for overgeneralization.

Effect of the Preparatory Course on the Frequency of Misconceptions

The analysis of the frequency of misconceptions revealed that misconceptions are encountered less frequently after the instruction. The effect sizes I report are large and significant for all the misconceptions with the lowest Cohen's *d* of all effects for the misconception that *intermolecular forces occur within molecules* (*d* = 0.81, see Table 35). This finding highlights the challenge students face in keeping covalent bonds apart from intermolecular forces.

Table 35: Comparison of Frequency of Misconceptions at Pre-Test and Post-Test

		Pre-Test			Post-Test			Cohen's *d*	
Misconception	Max	M	SD	FoM	M	SD	FoM	*d*	CI_{95}
Overgeneralization	21	7.72	4.02	0.37	2.23	2.39	0.11	1.64	**1.44; 1.83**
NaCl molecule	11	4.31	2.60	0.39	0.96	0.94	0.09	1.70	**1.48; 1.88**
Subunit or pairs in salts	6	2.08	1.24	0.35	0.38	0.70	0.06	1.66	**1.46; 1.86**
IMF in metals	3	1.66	1.06	0.55	0.16	0.54	0.05	1.75	**1.55; 1.94**
IMF in ionic compounds	2	0.99	0.82	0.50	0.11	0.35	0.06	1.38	**1.19; 1.57**
IMF within molecules	4	1.73	1.12	0.43	0.86	1.03	0.22	0.81	**0.63; 0.99**
Ionic lattice	1	0.82	0.39	0.82	0.07	0.26	0.07	2.24	**2.03; 2.46**
Metallic lattice	4	2.38	1.23	0.60	0.22	0.64	0.06	2.16	**1.95; 2.38**

Note. Max = maximum points, M = mean, SD = standard Deviation, FoM = frequency of misconception, IMF = intermolecular forces. Bolded values showcase which of the FoM values differed significantly between time points.

Comparing the frequency of misconception at post-test and follow-up (see Table 36) revealed that the *overgeneralization* misconception has increased at the follow-up time point with a small effect size (*d* = -0.21, paired *t*-test, *t*(206) = -2.18, *p* = .03, average difference = -0.28). Additionally, the *NaCl as a molecule* misconception is detected more frequently: There is a small but significant effect (*d* = -0.23, paired *t*-test, *t*(206) = -2.01, *p* = .05, average difference = -0.16).

Table 36: Comparison of Frequency of Misconception at Post-Test and Follow-up

		Post-Test			Follow-up			Cohen's *d*	
Misconception	Max	M	SD	FoM	M	SD	FoM	*d*	CI_{95}
Overgeneralization	21	2.23	2.39	0.11	2.77	2.65	0.13	**-0.21**	**-0.39; -0.03**
NaCl molecule	11	0.96	0.94	0.09	1.20	1.12	0.11	**-0.23**	**-0.41; -0.05**
Subunit or pairs in salts	6	0.38	0.70	0.06	0.42	0.77	0.07	-0.05	-0.22; 0.13
IMF in metals	3	0.16	0.54	0.05	0.25	0.67	0.08	-0.13	-0.31; 0.04
IMF in ionic compounds	2	0.11	0.35	0.06	0.12	0.40	0.06	-0.05	-0.23; 0.13
IMF within molecules	4	0.86	1.03	0.22	1.00	0.98	0.25	-0.14	-0.32; 0.04
Ionic lattice	1	0.07	0.26	0.07	0.06	0.24	0.06	0.03	-0.15; 0.21
Metallic lattice	4	0.22	0.64	0.06	0.24	0.68	0.06	-0.05	-0.22; 0.13

Note. Max = maximum points, M = mean, SD = standard Deviation, FoM = frequency of misconception, IMF = intermolecular force. Bolded values showcase which of the FoM values differed significantly between time points. Non-negligible, small effects sizes are highlighted in red.

The increased frequency of misconception of *overgeneralization* is in line with the finding of the changes concerning the subscore of the covalent and intermolecular forces. The increase in the *NaCl as a molecule misconception* frequency highlights how attractive it is for students to assume all matter is comprised of molecules with sodium chloride as a prominent example.

Analyzing Conceptual Change with a Sankey Plot

To investigate how misconceptions and mental representations of sodium chloride change over time and with the intervention, Item Q6 of the CBI (see Figure 14, p. 45) is investigated separately with a Sankey plot (see Figure 77). A large and sustainable shift from scientifically less correct models (synthetic and covalent models) toward the correct model was observed from the pre-test (left column) to post-test (middle column). Whereas about 10 % of students will fall back towards other models from the post-test to the follow-up test (right column), the same amount of students changed from other models towards the correct mental representation of sodium chloride. These findings support hypothesis 3 that students reduce the frequency of misconceptions significantly from pre- to post-test. Additionally, we observed that for misconceptions concerning ionic compounds the conceptual change is sustainable for many students when assessed one to two weeks later.

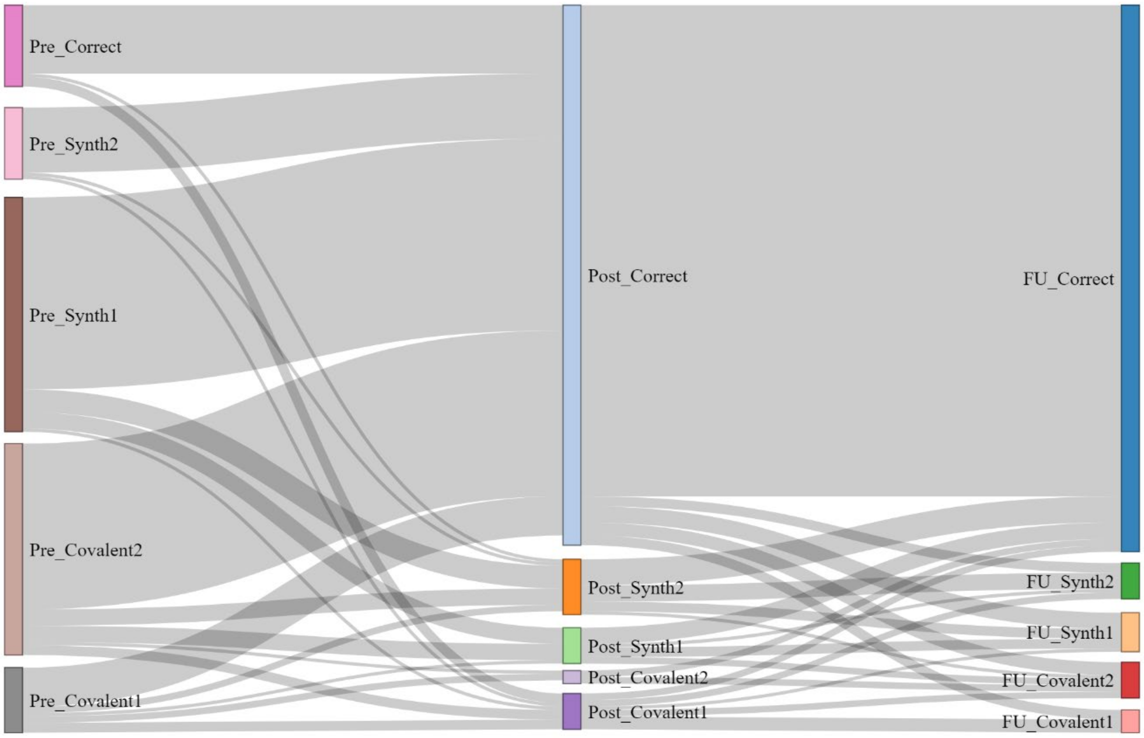


Figure 77: Sankey plot of item Q6 for the distribution of the preparatory students' mental representations at pre-test (left), at post-test (middle), and follow-up (right). From top to bottom; correct to least scientifically correct concept: Correct = accurate model of sodium chloride, Synth2 = synthetic model 2 (subunit representation), Synth1 = synthetic model 1 (ions but represented as molecules), Covalent2 = Sodium chloride as molecules made of neutral atoms, Covalent1 = neutral atoms in a lattice structure

6.4 Discussion

While controlling for the retest effect, the learning gains were significant and large after the intervention. Hence, the results strongly support the idea that conceptual change can also happen three to four years *after* students have learned about the concepts of chemical bonding models. While students before attending university still hold many misconceptions in regards to chemical bonds, it is this study's finding that students can improve in a short period of time with large effect sizes. While the conceptual understanding total scores went from one-third of the maximum total score to two-thirds in seven hours of instruction, the frequency of misconceptions was reduced with large effect sizes. While the students were able to keep a high level of conceptual understanding one to two weeks after the intervention a significant decrease with a small effect size was observed. Due to the strict time restraints, students were provided less time to actively construct their knowledge and make important inferences on their own. In line with the literature (e.g. Förtsch et al., 2017; Lombardi et al., 2021) this leads to less cognitive activation and possibly less sustainable learning gains. This may well be the reason why a small decrease in conceptual understanding was observed after just one to two weeks after the intervention. This interpretation is further supported by the findings of the Gymnasium intervention study, where students were given more time to work with the comparing and contrasting materials (see chapter 5). With this approach, even three months after the intervention the students were able to largely keep their level of conceptual understanding (with a significant decrease but with negligible effect size). While the results of these two studies are not perfectly comparable it still supports the idea that an initial comparing and contrasting introduction with more time at hand might be superior to a condensed preparatory course when it comes to the sustainability of the acquired conceptual understanding of chemical bonding models.

Still, the question remains, why is it that an intervention designed to foster students' first-time learning about chemical bonding is also so successful with students having already been instructed on the topic? On a first look, the two scenarios look very different: students learning about chemical bonding *for the first time* and students attending a *repetition course*. However, the reader should be cautious in seeing too many differences in these two cases: we cannot assume that students have never thought about matter being comprised of molecules before they enter the chemistry classroom for the first time. Students will bring a multitude of naïve theories to the classroom. And if they have not formed the misconceptions yet, who tells us that they do not form "attractive" deductions on the spot? This work's main finding is in fact that students do exactly that, and very often: overgeneralization is in our human nature. To simplify and infer things from the known to the unknown is a strong tool and has probably helped students navigate safely through daily life from a very young age. Why should they not keep on doing so when they are older? My point is that while the two situations do look very different, they are not. At both time points students will have misconceptions – maybe since their time in the Gymnasium or being made up on the spot, i.e. *in situ* preparation to use a chemical term. This study has also revealed something else: Whereas it is very interesting to find a way how to largely improve students' conceptual understanding in the aftermath of being instructed on the topic, it is at least as interesting to find out where students will fall back into old patterns and misconceptions. Such a finding can help guide chemistry educators to think more about where to invest more efforts to reduce such a fallback. The inventory I have developed has proven very helpful for the analysis of the decrease of conceptual understanding beyond the total scores. Using the concept *subscores* as a guidance to know what to look for as well as the *frequency of misconception* assessment tool helped to crystalize the fact that students are most strongly prone to go back to overgeneralize.

7 Conclusion and Implication for Future Research and Teaching Practices

This dissertation project had two overarching goals: (1) to address the need for the diagnosis of the understanding of the fundamental concept of chemical bonding, and (2) to present and evaluate options of how to foster conceptual understanding.

The first aim was addressed with the development of a new inventory on chemical bonding. The development of this inventory went hand in hand with first-year students' assessment of conceptual understanding of chemical bonding (chapter 2, *Piloting Phase* at Gymnasium and university and *University Studies 1 and 2*). After four years of development and four rounds of application (N = 2360), the *chemical bonding inventory* (CBI) is ready for use: The psychometric data of the inventory is good, the time of application is low (20 – 30 minutes) and there are additional assessment possibilities beyond the total score. I presented additional tools for a more detailed analysis of the data: with the use of *subscores*, representing the three bonding types and intermolecular forces, as well as the *frequency of misconception* measure. Those tools were useful in identifying five major challenges students typically encounter when learning about chemical bonding (see p. 40). The most prominent of all is the tendency of students to overgeneralize the covalent bonding type and all the characteristics of molecular substances (e.g. the presence of intermolecular forces). I detected multiple misconceptions in my investigations: Some of them replicating findings of other studies in other countries, e.g. the misconception of *sodium chloride as a molecule* idea. My findings are in line with previous research but also extend insights described in the literature. I further investigated the well-known *sodium chloride as a molecule* misconception and assessed facets of that misconception, describing synthetic models and even proposing a way how to observe the conceptual change with one single item (see p. 44 and p. 153 for a more detailed discussion). Additionally, I also report new facets of misconceptions and new misconceptions with a large cohort of students (N = 1946) that have either not been described or evaluated with such a sophisticated tool and so many participants giving a realistic and quantitative picture of the prevalence of the misconceptions held by Swiss science university students before attending lectures.

The identified challenges laid out the way how to tackle these observed misconceptions and how to best foster conceptual understanding of chemical bonding: Comparing and contrasting has been identified as a promising method of how to counteract students' strong tendency towards overgeneralization (see chapter 3). This finding was used together with the previously identified *five major challenges* (see chapter 2, p. 40) to formulate *five main ideas* that shaped the development of the comparing and contrasting teaching materials (see chapter 4). A stronger focus was laid on comparing the different bonding types. A major curriculum change was made by proposing to introduce the three bonding types simultaneously at the very beginning of the topic of chemical bonds and the implementation of early comparisons between the different types of bonding models. The process of developing new teaching materials was guided by multiple rounds of evaluation. The introduction of three concepts at once is not an easy feat. My evaluations in practice were necessary to find the appropriate degree of *difficulty* without overloading students cognitively. The teaching materials in the presented form are readily available for use in school settings, as has been confirmed by more than ten experienced chemistry teachers using the materials. Teaching materials for 23 – 24 lessons (on approximately 100 pages) were presented to foster students' conceptual understanding taking into account the previously stated major challenges and main ideas of how to best tackle them.

The teaching materials, and implicitly with it the method of comparing and contrasting, were evaluated for their effectiveness in advanced placement with the *Gymnasium intervention study (N* = 326, see chapter 5). The main research question was whether the comparing and contrasting method fostered conceptual understanding more strongly than conventional teaching methods. The findings were very clear in that aspect that in fact, students did learn significantly more with large effects evaluated at the post-test. The study revealed that the acquisition of knowledge was also sustainable, indicated by the high concept scores values even three months after the intervention. The lower frequency of misconception at follow-up compared to the control group is another indication of the effectiveness of the teaching materials in sustainably fostering conceptual understanding. There are clear signs that the awareness of the different bonding situations could be effectively fostered thus leading to a lower prevalence of misconceptions.

After the successful application of the teaching materials at the Gymnasium level, I was interested in whether the material could also be used for a short preparatory course (7 lessons) to improve students' understanding after they were previously instructed on the topic of chemical bonding. In the *university intervention study* (*N* = 293) I found that students can significantly increase their understanding using the developed material and with large effect sizes. However, there are signs that it might make a difference concerning the longevity of the acquired conceptual understanding if the topic is introduced in this condensed version (small but significant effect for a lowering of the understanding after one to two weeks after the intervention).

Overall, I can state that I have designed and evaluated an appropriate assessment tool for the identification of the major challenges for the understanding of chemical bonding, helped develop and optimize a teaching unit that was very successful when applied in a classroom intervention study, and designed a preparatory course that fostered university students' understanding before the start of their studies.

7.1 Limitations

What are the limitations of the presented research? Because there was no inventory available to use as a pre-test or post-test I had to design the inventory to assess conceptual understanding on my own. I would have, of course, preferred to use an external assessment tool for the intervention I came up with. However, I designed the *Chemical Bonding Inventory* not primarily as a tool to assess future interventions but to assess the conceptual understanding of university students at the start of their studies in general. I am convinced that the new inventory is useful beyond the assessment of the interventions conducted in this study and has high content validity.

The author has been part of the *Gymnasium intervention study* as one of the teachers in the intervention group. With that, I am the only teacher knowing the exact content of the tests and could have (in theory) taught students to the test. I have of course not intentionally done so, as was confirmed by the chemistry teacher who was sitting in class during the whole intervention. Additionally, the main findings of this study have also been assessed without the students whom I have instructed and found that the effects slightly decreased but remained strong. This was to be excepted since my students only make up about 10 % of the intervention group.

The results suggest that the developed comparing and contrasting teaching materials foster conceptual understanding more strongly *than conventional instruction*. This finding has of course the more relevance the higher the quality of the conventional teaching was. I am convinced that the instruction the comparing and contrasting approach has been compared to was above the Swiss average since the teachers involved in the study were all long-time practitioners (and many of them teacher trainers) with well-worked out teaching materials and were used to optimally teach with their own materials. The teachers who participated were all genuinely interested in learning about new ways of how to teach this complex topic, which is normally a sign of competence for educators. Additionally, the teachers were informed about common misconceptions (without directly telling them how I assess them) and knew more than they would have if the intervention study would have been set up as a waiting group design. First, this had been the plan, but the Covid-19 pandemic changed my plans. After all, I was strongly working against the intervention with such a setup and decided for the setup in parallel classes to mitigate the teacher effect during the intervention.

For my study assessing the effectiveness of the preparatory course, no active control group was set up. The increase of conceptual understanding and reduction of misconception in comparison to before the intervention has of course standing since I have controlled for re-test effects, but other interventions that might have similar or stronger effects may exist. However, since there were no preparatory courses in chemistry at ETH Zurich, there was no apparent control group that was available.

7.2 Implication for Teaching and Future Research

Chemistry educators are faced with students' misconceptions in the classroom on a regular basis. Many chemistry teachers I came in contact with, were aware of the main finding of this project: Students have difficulties when it comes to the differentiation between the bonding types. Many were also aware of the molecule misconception. My research helped to quantify those observations which a large dataset. I have also described misconceptions that were not as present in many teachers' minds (e.g. the lattice misconceptions, and the existence of intermolecular forces within metals, to name two). The general catalog for the major challenges and most prominent misconceptions will hopefully influence future teaching in chemistry classes. Making chemistry teachers aware of such findings might help to focus students' attention on those difficulties in the future. I have not only shown where the difficulties lie but I also present classroom-evaluated and ready-to-use teaching materials that have the potential to sustainably foster students' conceptual understanding of chemical bonding. The teaching materials' effectiveness has been assessed with the *Gymnasium intervention study*: The developed teaching materials were very effective in fostering conceptual understanding compared to conventional teaching materials. The developed teaching material is made accessible to chemistry teachers and will hopefully influence teaching about chemical bonding in the future.

The method of comparing and contrasting with a simultaneous introduction of *three concepts at once* has been investigated for their effectiveness in a classroom setting compared to a sequential introduction. Whereas the simultaneous introduction of *two* concepts has been investigated in the context of mathematics instruction (Ziegler & Stern, 2014, 2016), this research is the first to show that a comparing and contrasting introduction can be more effective than the sequential introduction of three concepts.

The full inventory has 25 items and takes about 20 to 30 Minutes to complete. The large dataset might help to potentially identify items with the highest loadings to develop a shortened version of the inventory without losing too much validity. Wright Mapping is of particular interest in that aspect.

When looking at newly enrolled university students' conceptual understanding subscores of chemical bonding, the primary profile analysis did not yield profiles worth investigating further. However, an in-depth analysis of the misconceptions students hold might be of more interest. There are more interesting things to investigate in the intervention samples: The analysis of the frequencies of misconceptions in the *university intervention sample* from post-test to follow-up has shown that certain misconceptions were more prone to reappear. Are there profiles of interest for the *Gymnasium intervention sample*? Do students learn and or forget about the different bonding types differently? Analysis over time points with a focus on individual profiles might shed more light on these questions.

Furthermore, students in the control group of the *Gymnasium intervention study* improve from post-test to follow-up. A more detailed analysis of the conceptual understanding subscores and frequencies of misconceptions might shed more light on the topic. Additionally, I could investigate which classes have improved more and talk to those teachers about their teaching methods after the instruction on chemical bonding.

The insights I gathered during my dissertation project fostered the impression that the method of comparing and contrasting might be especially useful in fostering students' conceptual understanding in the field of *chemistry education* since chemical concepts often appear to be similar on the surface. As stated in the introduction, one of the particularities of chemistry is that we can never really observe processes on the atomic level and that the language we use to describe the different substances is always the same even though they might represent completely different classes of substances. It might be worth having a prolonged look at the chemistry curriculum to investigate where similar difficulties as with the topic of chemical bonding models might be observed. More advanced topics like *coordination chemistry* (e.g. interactions between anionic or neutral ligands and the coordination center in transition metal complexes compared to ionic or covalent bonding) or the topic of *acids and bases* (e.g. comparing weak and strong acids respectively bases) might be of particular interest.

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Illustrations

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9 Appendix

Appendix 1: Inventories

Appendix 1.1: Chemical Bonding Inventory (CBI)

The chemical bonding inventory (CBI) as a commented print-out version is shown on the following pages.

Chemical Bonding Inventory (CBI)

Print-out version

Wichtige Hinweise:

Der Fragebogen wird **ohne Namen und anonym erhoben.** Damit eine Zuweisung von Vortest zum Nachtest möglich ist, müssen Sie jedoch zweimal den gleichen Code generieren.

Persönlicher Code:

(1)	(2)	(3)	(4)	(5)

(1) Anfangsbuchstabe des Vornamens Ihrer Mutter *(z. B.* ***N****ina = N)*

(2) Ihr Geburtsmonat als **zweistellige** Zahl *(z. B. Oktober = 10)*

(3) Letzter Buchstabe des Vornamens Ihres Vaters (*z.B. Herber****t*** *= T*)

(4) Ihr Jahrgang als zweistellige Zahl (*z.B. 2004 = 04*)

(5) Ihr Geschlecht *(****W*** *für weiblich,* ***M*** *für männlich,* ***D*** *für divers)*

Kreuzen Sie jeweils **bei jeder Antwortmöglichkeit** die richtige Option an (korrekt oder falsch). Es kann bei jeder Frage **mehr als eine Antwort korrekt sein.**

Beispiel: ☐ korrekt ☒ falsch

Q1: Wir betrachten einen Salzkristall (NaCl). In welcher Weise liegen Natrium und Chlor in dieser Verbindung vor?

☐ korrekt ☐ falsch als neutrale Natriumatome und neutrale Chloratome

☐ korrekt ☐ falsch als Natrium-Chlorid-Moleküle

☐ korrekt ☐ falsch als Natriumionen und Chloridionen

Q2: Was ist die ursächliche Erklärung dafür, dass zwischen Natrium und Chlor Bindungen zustande kommen?

Die Bindung entsteht…

☐ korrekt ☐ falsch da Natrium von sich aus die Tendenz hat, Elektronen abzugeben.

☐ korrekt ☐ falsch weil die Anziehung von Na^+ und Cl^- energetisch vorteilhaft ist.

☐ korrekt ☐ falsch weil Natrium ein Elektron auf Chlor überträgt.

☐ korrekt ☐ falsch weil Natrium und Chlor ein Elektron teilen.

Q3: Wovon hängt es ab, ob man einen Atomverband als Molekül bezeichnet?

Es ist entscheidend, …

☐ korrekt ☐ falsch wie viele Atome miteinander verbunden sind (mindestens zwei).

☐ korrekt ☐ falsch welche Bindungsarten zwischen den Atomen vorkommen.

☐ korrekt ☐ falsch ob Atome in einem geladenen oder ungeladenen Zustand vorliegen.

☐ korrekt ☐ falsch dass unterschiedliche Elemente vorkommen.

☐ korrekt ☐ falsch welche Atomsorten (metallische/nichtmetallische) vorkommen.

Q4: Lithiumbromid, eine Ionenverbindung, wird mit der chemischen Formelschreibweise LiBr dargestellt. Welche Schlüsse lassen sich aus dieser Formel ziehen?

☐ korrekt ☐ falsch Die Schreibweise lässt den Schluss zu, dass Lithium- und Bromatome jeweils als Paare zu zweit miteinander verknüpft sind.

☐ korrekt ☐ falsch Die Schreibweise gibt Auskunft darüber, aus welchen Atomsorten der Stoff aufgebaut ist.

☐ korrekt ☐ falsch Die Schreibweise lässt einen Schluss zu, welche Untereinheiten in diesem Feststoff gebildet werden.

☐ korrekt ☐ falsch Die Schreibweise gibt Auskunft darüber, in welchem Verhältnis die Atomsorten im Stoff vorkommen.

Q5: Bei Raumtemperatur zerfällt eine Aluminiumfolie nicht spontan in ihre Atome. Welche der folgenden Begründungen sind korrekt?

☐ korrekt ☐ falsch Die Atome sind bei Raumtemperatur durch feste Gitter verbunden.

☐ korrekt ☐ falsch Durch das Ausbilden kovalenter Bindungen werden die Atome zusammengehalten.

☐ korrekt ☐ falsch Die Anziehung zwischen dem Elektronengas und den Atomrümpfen hält den Atomverband zusammen.

☐ korrekt ☐ falsch Zwischen den Atomen bestehen zwischenmolekulare Kräfte, die die Folie zusammenhalten.

☐ korrekt ☐ falsch Durch das Abgeben der Valenzelektronen entstehen Aluminiumkationen. Diese werden durch das Ionengitter zusammengehalten.

Q6: Natrium und Chlor reagieren zusammen zu Natriumchlorid (NaCl). Welche der folgenden Aussagen treffen zu?

☐ korrekt ☐ falsch Es bilden sich Natriumionen und Chloridionen, welche sich aufgrund der unterschiedlichen Ladungen gegenseitig anziehen.

☐ korrekt ☐ falsch Neutrale Natriumatome und neutrale Chloridatome lagern sich in einer gitterartigen Struktur zusammen.

☐ korrekt ☐ falsch Natrium- und Chloratome bilden Elektronenpaarbindungen aus, um Natriumchlorid-Moleküle zu bilden.

☐ korrekt ☐ falsch Es bilden sich Natriumionen und Chloridionen, welche sich zu Natriumchlorid-Molekülen zusammenschliessen.

☐ korrekt ☐ falsch Jeweils ein Natriumion und ein Chloridion schliessen sich zu einer Einheit zusammen.

Q7: Welche Eigenschaften treffen auf Ionen zu?

☐ korrekt ☐ falsch Ionen sind elektrisch neutral.

☐ korrekt ☐ falsch Die Gesamtladung eines Ions ist Null.

☐ korrekt ☐ falsch Ionen sind stets negativ geladen.

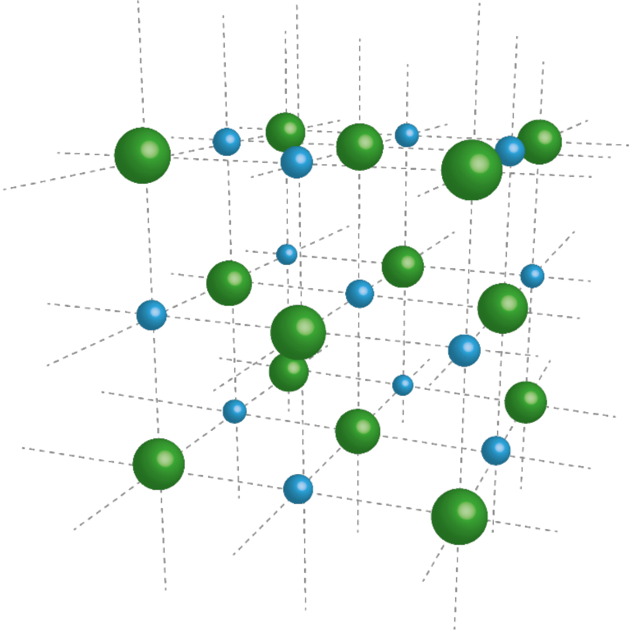
☐ korrekt ☐ falsch Ionen sind stets positiv geladen.

☐ korrekt ☐ falsch Ionen sind positiv oder negativ geladen.

Q8: Die unten dargestellte Abbildung stellt einen Ausschnitt aus einem Kaliumchlorid-Kristall dar. In dieser Verbindung sind die Ionen in einer Gitterstruktur angeordnet (gestrichelte Linien).

Q8.1 Kaliumchlorid wird mit der chemischen Formelschreibweise KCl dargestellt. Entsprechen dieser Schreibweise im Feststoff klar definierte Paare?

☐ korrekt ☐ falsch Es gibt klar definierte Paare.



Q8.2 Was hält die Ionen im Kristallgitter auf ihren Positionen?

☐ korrekt ☐ falsch die zwischenmolekularen Kräfte

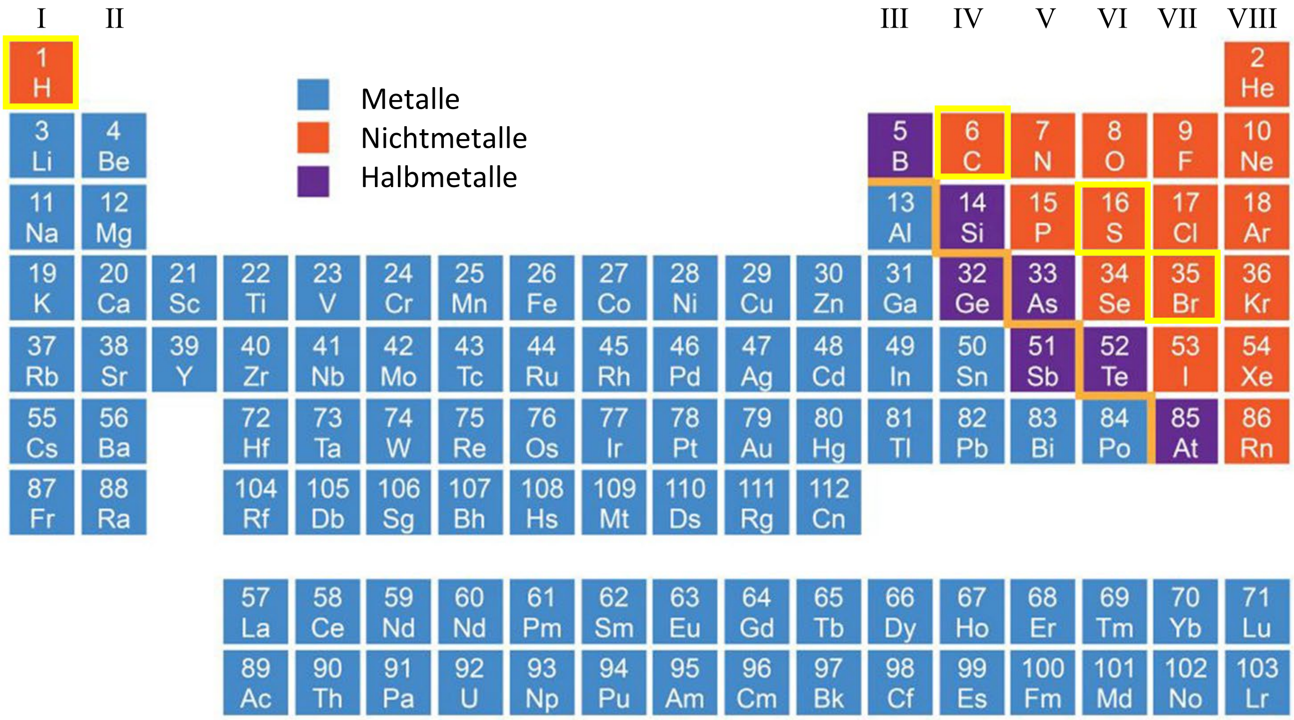
☐ korrekt ☐ falsch das Ionengitter

☐ korrekt ☐ falsch die gebildeten kovalenten Bindungen

☐ korrekt ☐ falsch das Elektronengas

☐ korrekt ☐ falsch die Anziehungs- und Abstossungskräfte der Ionen

Q9/Q10: Unten stehend finden Sie ein Periodensystem, welches Sie für das Lösen der folgenden Aufgaben verwenden können.



Element	**Anzahl an Valenzelektronen**	**Typische Anzahl an Bindungen zu anderen Atomen in einem Molekül.**
Beispiel: H	***1***	***1***
S		
Br		
C		

Q9

Q10

Q11: Kreuzen Sie die richtige Bezeichnung für die folgenden Stoffe an.

Summenformel	Metall	ionische Verbindung	Molekül	Anion	Kation
PH_3					
NaCl					
NH_4^+					
LiF					
C_2H_6					
K					
$BeBr_2$					
CO_2					
HCO_3^-					

Q12: Kupfer ist ein Metall. Welche der folgenden Aussagen treffen auf die Bindungen in einem Metallblock aus Kupfer zu?

☐ korrekt ☐ falsch Es kommen Elektronenpaarbindungen vor.

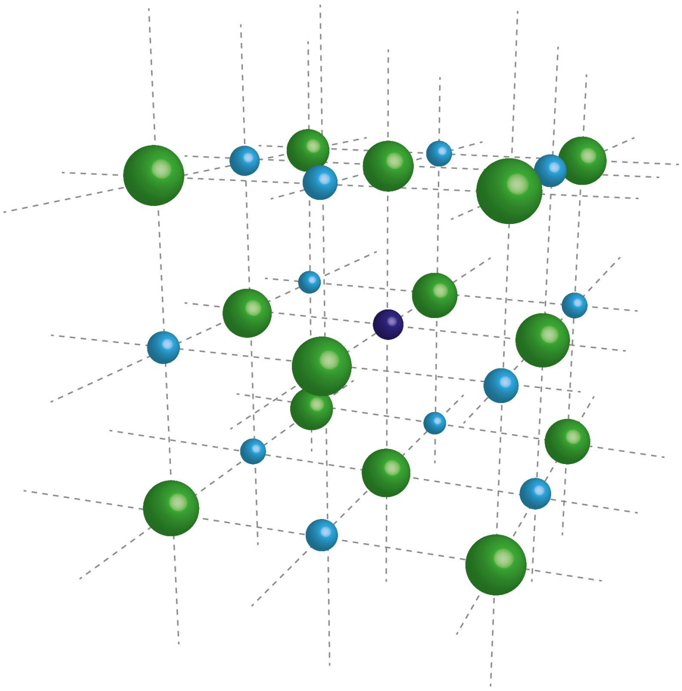
☐ korrekt ☐ falsch Die Atome liegen als positiv und negativ geladene Ionen vor.

☐ korrekt ☐ falsch Die Metallatome werden durch zwischenmolekulare Kräfte zusammengehalten.

☐ korrekt ☐ falsch Die Bindungen in Kupfer sind von ionischen als auch kovalenten Bindungen verschieden.

Q13: Die unten dargestellte Abbildung stellt einen Ausschnitt aus einem Kaliumchlorid-Kristall (KCl) dar. In dieser Verbindung sind die Ionen in einer Gitterstruktur angeordnet (gestrichelte Linien). Wie viele Bindungspartner besitzt das in dunkelblau hervorgehobene Kalium-Ion?

- ☐ 1
- ☐ 4
- ☐ 6
- ☐ 14
- ☐ unbestimmt viele



Q14: Aluminiumatome besitzen dreizehn Elektronen, wovon drei als Valenzelektronen bezeichnet werden. Welche der folgenden Aussagen über Valenzelektronen treffen zu, wenn wir Aluminiumatome in einem Stück Aluminium betrachten?

☐ korrekt ☐ falsch Sämtliche Valenzelektronen eines Aluminiumatoms werden abgegeben.

☐ korrekt ☐ falsch Die abgegebenen Valenzelektronen verlassen das Metallstück, womit die positiv geladenen Atomrümpfe zurückbleiben.

☐ korrekt ☐ falsch Die Valenzelektronen werden in das Elektronengas abgegeben.

☐ korrekt ☐ falsch Einige Aluminiumatome nehmen Valenzelektronen auf, während andere Valenzelektronen abgeben.

☐ korrekt ☐ falsch Die Valenzelektronen werden an direkt benachbarte Atomkerne abgegeben.

Q15: Wir betrachten ein Stück Kupfer. Die Kupferatome sind darin in einem Metallgitter angeordnet. Welche Aussagen über das Metallgitter sind korrekt?

☐ korrekt ☐ falsch Das Metallgitter hält die Atome zusammen.

☐ korrekt ☐ falsch Das Metallgitter beschreibt die geometrische Anordnung der Atome.

☐ korrekt ☐ falsch Das Metallgitter ist eine eigenständige Struktur, welche Kupfer Stabilität verleiht.

☐ korrekt ☐ falsch Das Metallgitter hält die Atome auf ihren Positionen.

☐ korrekt ☐ falsch Das Metallgitter ergibt sich durch die Anordnung der Atome.

Q16: Welche Bindungsarten halten die Atome eines Moleküls zusammen?

☐ korrekt ☐ falsch kovalente Bindungen

☐ korrekt ☐ falsch Van-der-Waals Wechselwirkungen

☐ korrekt ☐ falsch metallische Bindungen

☐ korrekt ☐ falsch ionische Bindungen

☐ korrekt ☐ falsch Wasserstoffbrückenbindungen

☐ korrekt ☐ falsch zwischenmolekulare Kräfte

Q17: Zwischenmolekulare Kräfte wirken …

☐ korrekt ☐ falsch in metallischen Stoffen.

☐ korrekt ☐ falsch zwischen Molekülen.

☐ korrekt ☐ falsch in Salzen (ionischen Verbindungen).

☐ korrekt ☐ falsch zwischen Einzelatomen von Edelgasen.

Q18: Die zwischenmolekularen Kräfte sind typischerweise …

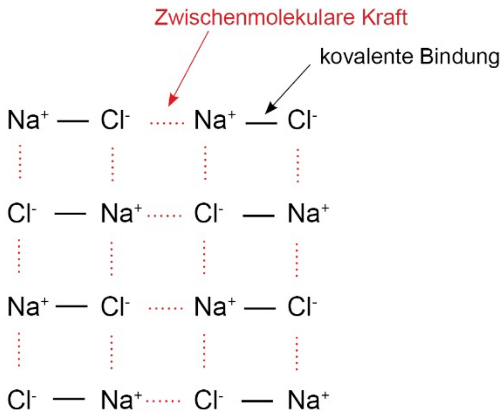
☐ kleiner ☐ gleich stark ☐ grösser wie kovalente Bindungen.

☐ kleiner ☐ gleich stark ☐ grösser wie die metallische Bindung.

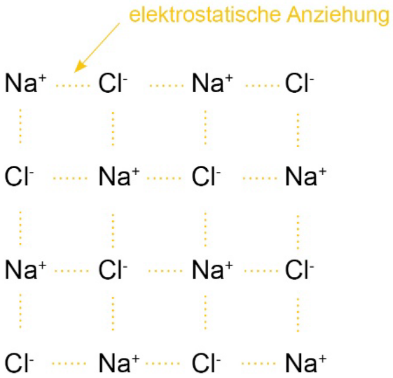
☐ kleiner ☐ gleich stark ☐ grösser wie die ionische Bindung.

Q19: Untenstehend sind vier Modelle eines Salzkristalls (NaCl) dargestellt. Welches der Modelle stellt die Bindungssituation in einem Salzkristall am besten dar?

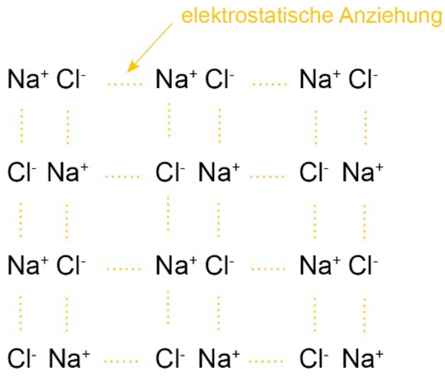
A



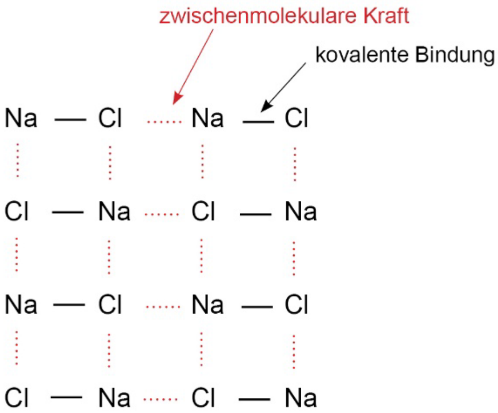
B



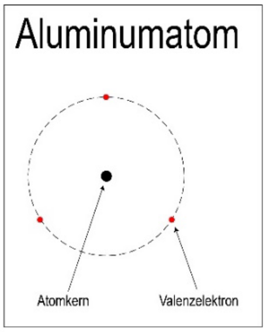
C



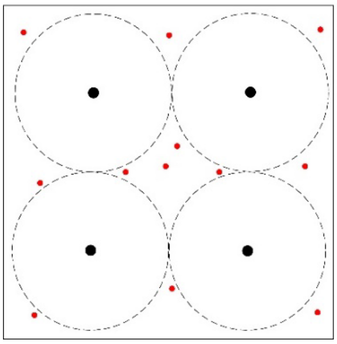
D



Q20: Nachfolgend ist ein isoliertes Aluminiumatom illustriert. Welche Darstellung illustriert am besten, wie die Atome im gebundenen Zustand vorliegen zum Beispiel in einer Aluminiumfolie.



A.



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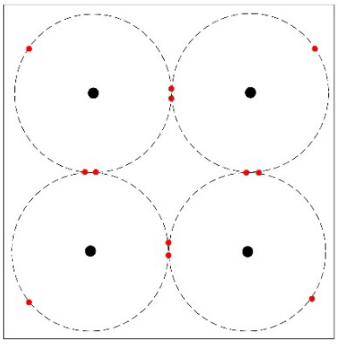
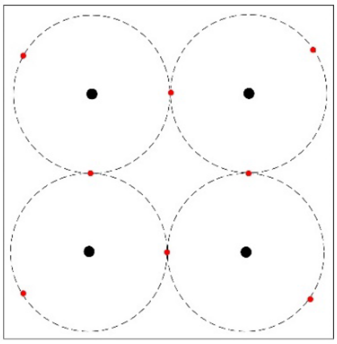


C.



Q21: Wassermoleküle (H_2O) zerfallen bei Raumtemperatur nicht in einzelne Atome. Welche Begründungen für das Zusammenhalten der Atome in einem Wassermolekül sind korrekt?

☐ korrekt ☐ falsch Die gebildeten Wasserstoffbrücken führen dazu, dass die Atome in den Wassermolekülen zusammenbleiben.

☐ korrekt ☐ falsch Die kovalenten Bindungen halten die Atome in den Wassermolekülen zusammen.

☐ korrekt ☐ falsch Die Anziehung von H^+ und O^{2-} führt dazu, dass die Atome der Wassermoleküle zusammenbleiben.

☐ korrekt ☐ falsch Die wirkenden Van-der-Waals-Kräfte halten die Atome der Wassermoleküle zusammen.

☐ korrekt ☐ falsch Die Dipol-Dipol-Wechselwirkungen halten die Atome der Wassermoleküle zusammen.

Q22: Eine Verbindung mit der Summenformel XY besteht aus zwei verschiedenen Atomsorten X und Y.

Fall 1: Die Verbindung XY ist ein ***Molekül*** und X ist ein *nichtmetallisches* Element: Dann ist Y ein ...

☐ metallisches Element

☐ nichtmetallisches Element

☐ metallisches oder nichtmetallisches Element.

Fall 2: Die Verbindung XY ist ein ***metallischer Stoff*** und X ist ein *metallisches* Element: Dann ist Y ein ...

☐ metallisches Element

☐ nichtmetallisches Element

☐ metallisches oder nichtmetallisches Element.

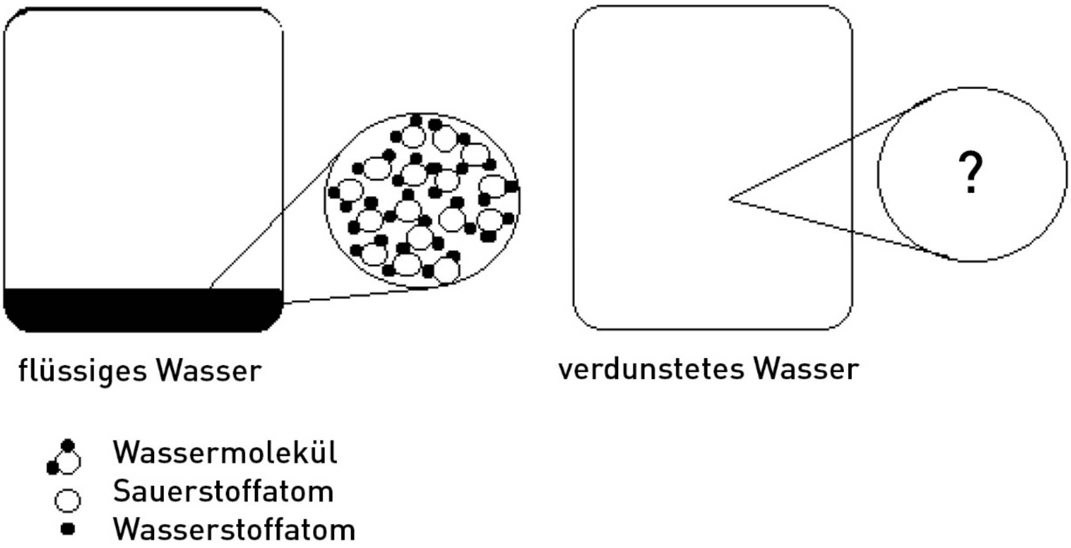
Fall 3: Die Verbindung XY ist ein ***Salz*** und X ist ein *metallisches* Element: Dann ist Y ein ...

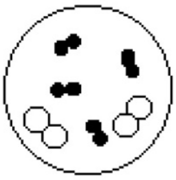
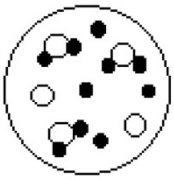
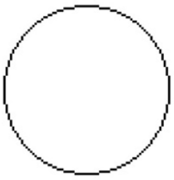
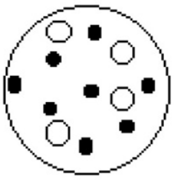
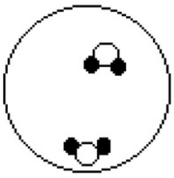
☐ metallisches Element

☐ nichtmetallisches Element

☐ metallisches oder nichtmetallisches Element.

Q23: Der Kreis auf der linken Seite zeigt eine vergrösserte Ansicht einer ganz kleinen Menge flüssigen Wassers in einem geschlossenen Gefäss. Was würde die vergrösserte Ansicht zeigen, nachdem das Wasser verdunstet ist? Wählen Sie eine der unten aufgeführten Optionen aus.



☐ ☐ ☐ ☐ ☐

Q24: Ordnen Sie die folgenden sechs Stoffe nach aufsteigenden Siedetemperaturen.

HCl, $CaCl_2$, H_2, H_2O, Ca, CH_3OH

tiefste Siedetemperatur 1.

2.

3.

4.

5.

höchste Siedetemperatur 6.

Q25: Um die sechs Stoffe in den gasförmigen Aggregatzustand zu bringen, muss den Kräften und/oder Bindungen, die die Stoffe zusammenhalten, entgegengewirkt werden.

Beurteilen Sie für jeden Stoff einzeln, ob und welche Bindungen gebrochen werden und/oder welchen Kräften entgegengewirkt werden muss, um diesen <u>Stoff gasförmig</u> werden zu lassen. Setzen Sie in der Tabelle für Zutreffendes Kreuze (mehrere pro Zeile möglich).

Stoff	**Kovalente Bindungen** werden gebrochen.	**Metallische Bindungen** werden gebrochen.	**Ionische Bindungen** werden gebrochen.	**Van-der-Waals-Kräften** wird entgegengewirkt.	**Wasserstoff-brücken** werden gelöst.	**Dipol-Dipol-Kräften** wird entgegengewirkt.
HCl						
$CaCl_2$						
H_2						
H_2O						
Ca						
CH_3OH						

Vortest zur chemischen Bindungslehre

CBI pre-test

Wichtige Hinweise:

Der Fragebogen wird **ohne Namen und anonym erhoben.** Damit eine Zuweisung von Vortest zum Nachtest möglich ist, müssen Sie jedoch zweimal den gleichen Code generieren.

Persönlicher Code:

(1)	(2)	(3)	(4)	(5)

(1) Anfangsbuchstabe des Vornamens Ihrer Mutter *(z. B. **N**ina = N)*

(2) Ihr Geburtsmonat als **zweistellige** Zahl *(z. B. Oktober = 10)*

(3) Letzter Buchstabe des Vornamens Ihres Vaters (*z.B. Herber**t** = T*)

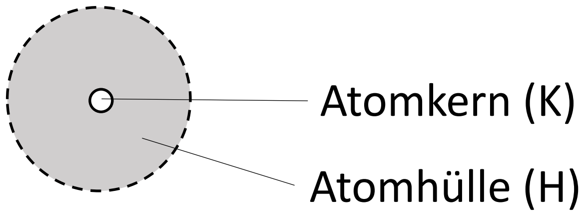
(4) Ihr Jahrgang als zweistellige Zahl (*z.B. 2004 = 04*)

(5) Ihr Geschlecht *(**W** für weiblich, **M** für männlich, **D** für divers)*

Kreuzen Sie jeweils **bei jeder Antwortmöglichkeit** die richtige Option an (korrekt oder falsch). Es kann bei jeder Frage **mehr als eine Antwort korrekt sein.**

Beispiel: ☐ korrekt ☒ falsch

P1 Die Abbildung illustriert ein Atom mit Atomkern (K) und Atomhülle (H).



a. Im Atomkern (K) befinden sich typischerweise folgende Elementarteilchen:

☐ korrekt ☐ falsch Elektronen

☐ korrekt ☐ falsch Protonen

☐ korrekt ☐ falsch Neutronen

☐ korrekt ☐ falsch Ionen

b. In der Atomhülle (H) befinden sich typischerweise folgende Elementarteilchen:

☐ korrekt ☐ falsch Elektronen

☐ korrekt ☐ falsch Protonen

☐ korrekt ☐ falsch Neutronen

☐ korrekt ☐ falsch Ionen

P2a–c Treffen die Aussagen auf die verschiedenen Elementarteilchen zu?

Trifft auf folgende Elementarteilchen zu:	**Elektronen**		**Protonen**		**Neutronen**	
	Ja	Nein	Ja	Nein	Ja	Nein
Weist eine positive elektrische Ladung auf						
Weist eine negative elektrische Ladung auf						
Weist keine elektrische Ladung auf						
Wird von Protonen abgestossen						
Wird von Neutronen abgestossen						
Wird von Elektronen abgestossen						

P3 Wie bezeichnet man ein Atom, dem ein Elektron entfernt wurde?

☐ korrekt ☐ falsch Es wird als Ion bezeichnet.

☐ korrekt ☐ falsch Es wird als Anion bezeichnet.

☐ korrekt ☐ falsch Es wird als Kation bezeichnet.

☐ korrekt ☐ falsch Es wird als Isotop bezeichnet.

P4/Q7 Welche Eigenschaften treffen auf Ionen zu?

☐ korrekt ☐ falsch Ionen sind elektrisch neutral.

☐ korrekt ☐ falsch Die Gesamtladung eines Ions ist Null.

☐ korrekt ☐ falsch Ionen sind stets negativ geladen.

☐ korrekt ☐ falsch Ionen sind stets positiv geladen.

☐ korrekt ☐ falsch Ionen sind positiv oder negativ geladen.

P5 Beschreiben Sie in eigenen Worten, wie Sie sich den Aufbau eines Salzkristalles (NaCl), bestehend aus den Elementen Natrium und Chlor, vorstellen? Sie dürfen auch eine beschriftete Skizze Ihrer Vorstellung anfertigen.

P6/Q1 Wir betrachten einen Salzkristall (NaCl). In welcher Weise liegen Natrium und Chlor in dieser Verbindung vor?

☐ korrekt ☐ falsch als neutrale Natriumatome und neutrale Chloratome

☐ korrekt ☐ falsch als Natrium-Chlorid-Moleküle

☐ korrekt ☐ falsch als Natriumionen und Chloridionen

P7 Unter der ersten Ionisierungsenergie eines Atoms versteht man die Energie, die aufgewendet werden muss, …

☐ korrekt ☐ falsch … um der Elektronenhülle eines Atoms ein Elektron zu entfernen.

☐ korrekt ☐ falsch … um der Elektronenhülle eines Atoms ein zusätzliches Elektron hinzuzufügen.

☐ korrekt ☐ falsch … um ein Atom in ein Ion mit positiver oder negativer Ladung umzuwandeln.

☐ korrekt ☐ falsch … um ein Atom in ein positiv geladenes Ion umzuwandeln.

P8/Q3 Wovon hängt es ab, ob man einen Atomverband als Molekül bezeichnet?

☐ korrekt ☐ falsch Es ist entscheidend, dass mehrere Atome miteinander verbunden sind.

☐ korrekt ☐ falsch Es ist entscheidend, welche Bindungsarten zwischen den Atomen vorkommen.

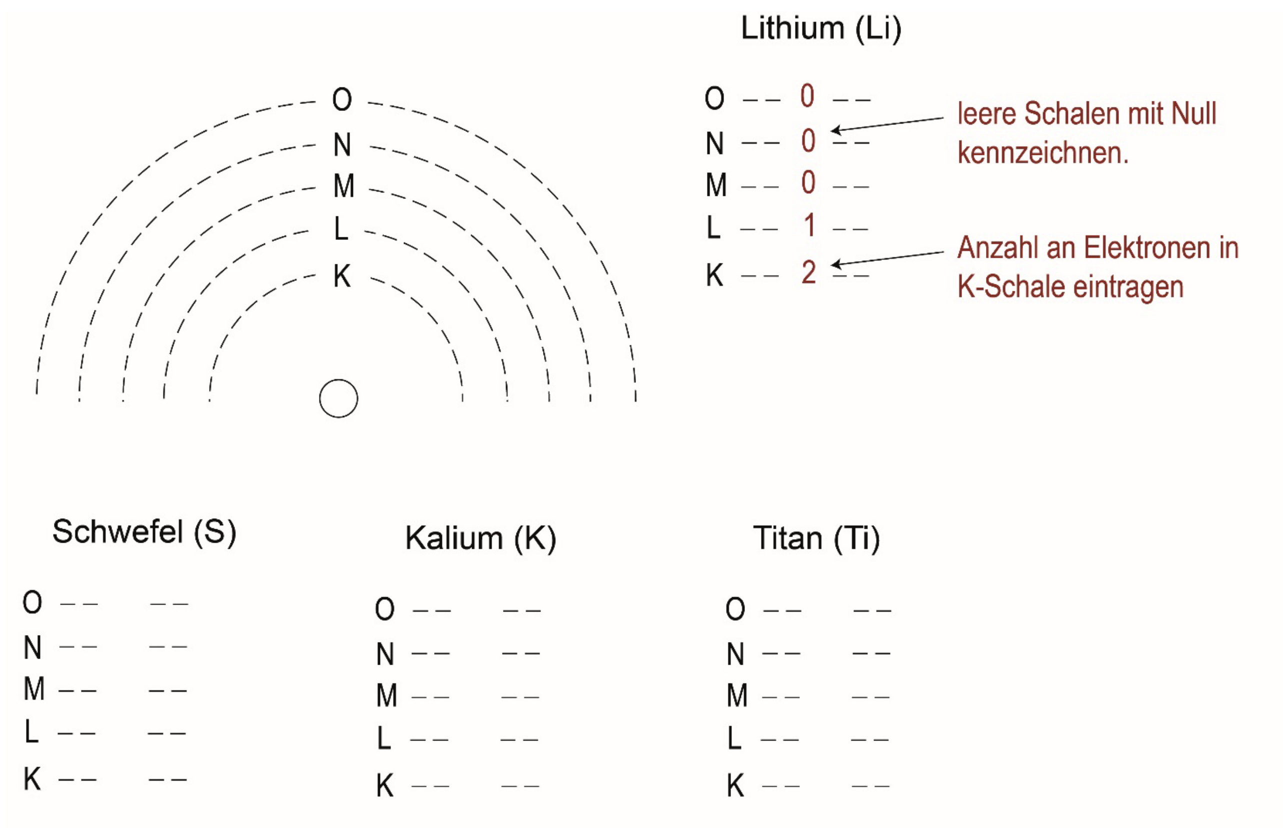
☐ korrekt ☐ falsch Es ist entscheidend, ob Atome in einem geladenen oder ungeladenen Zustand vorliegen.

☐ korrekt ☐ falsch Es ist entscheidend, dass unterschiedliche Elemente vorkommen.

☐ korrekt ☐ falsch Es spielt eine Rolle, welche Atomsorten (metallische/nichtmetallische) vorkommen.

P9 Was ist der Grund dafür, dass eine Aluminiumfolie nicht spontan in Aluminiumatome zerfällt?

P10 Im Chemieunterricht haben Sie bestimmt das Schalenmodell von Atomen kennengelernt. Geben Sie für die unten aufgeführten Elemente (S, K und Ti) für jede der angegebenen Schalen (K bis O) an, wie viele Elektronen sich darin befinden. Benutzen Sie dazu das zusätzlich ausgeteilte Periodensystem.



leere Schalen mit Null kennzeichnen.

Anzahl an Elektronen in K-Schale eintragen

P11/Q9 Wie viele Valenzelektronen besitzt …

A. Schwefel (S)?

B. Kalium (K)?

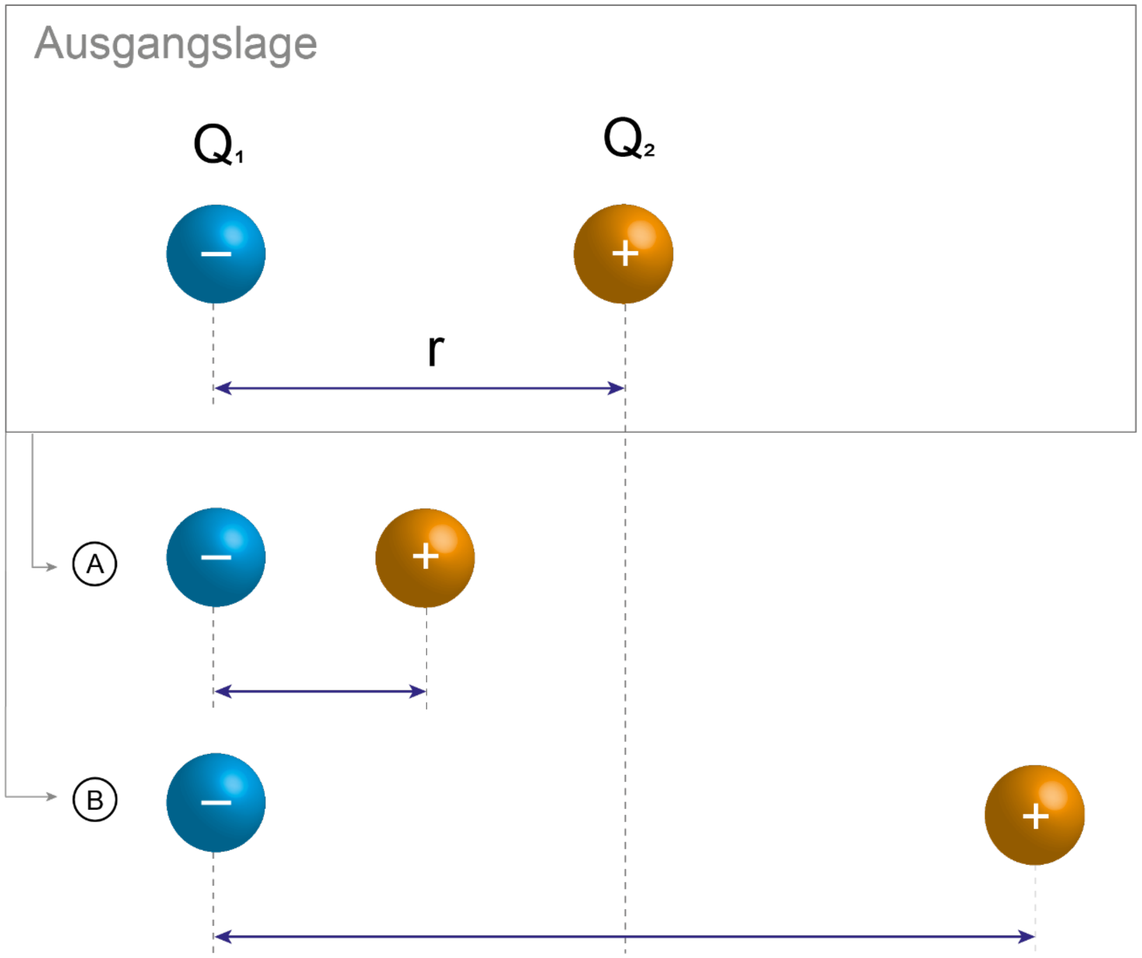
C. Brom (Br)?

D. Kohlenstoff (C)?

P12/Q4 Lithiumbromid, eine Ionenverbindung, wird mit der chemischen Formelschreibweise LiBr dargestellt. Welche Schlüsse lassen sich aus dieser Formel ziehen?

☐ korrekt	☐ falsch	Die Schreibweise lässt den Schluss zu, dass Lithium- und Bromatome jeweils als Paare zu zweit miteinander verknüpft sind.
☐ korrekt	☐ falsch	Die Schreibweise gibt Auskunft darüber, aus welchen Atomsorten der Stoff aufgebaut ist.
☐ korrekt	☐ falsch	Die Schreibweise lässt einen Schluss zu, welche Untereinheiten in diesem Feststoff gebildet werden.
☐ korrekt	☐ falsch	Die Schreibweise gibt Auskunft darüber, in welchem Verhältnis die Atomsorten im Stoff vorkommen.

P13 In der untenstehenden Abbildung finden Sie zwei Ladungen Q_1 und Q_2 im Abstand r.



a. Im Fall A wird der Abstand r zwischen den Ladungen im Vergleich zur Ausgangslage halbiert, während die Ladungen gleich bleiben. Dabei verändert sich die Stärke der Coulombkraft F wie folgt:

☐ korrekt ☐ falsch Die Kraft ist noch ein Viertel der ursprünglichen.

☐ korrekt ☐ falsch Die Kraft halbiert sich.

☐ korrekt ☐ falsch Die Kraft verdoppelt sich.

☐ korrekt ☐ falsch Die Kraft verändert sich nicht.

☐ korrekt ☐ falsch Die Kraft wird vervierfacht.

b. Im Fall B wird der Abstand r zwischen den Ladungen im Vergleich zur Ausgangslage verdoppelt, während die Ladungen gleich bleiben. Dabei verändert sich die Stärke der Coulombkraft F wie folgt:

☐ korrekt ☐ falsch Die Kraft ist noch ein Viertel der ursprünglichen.

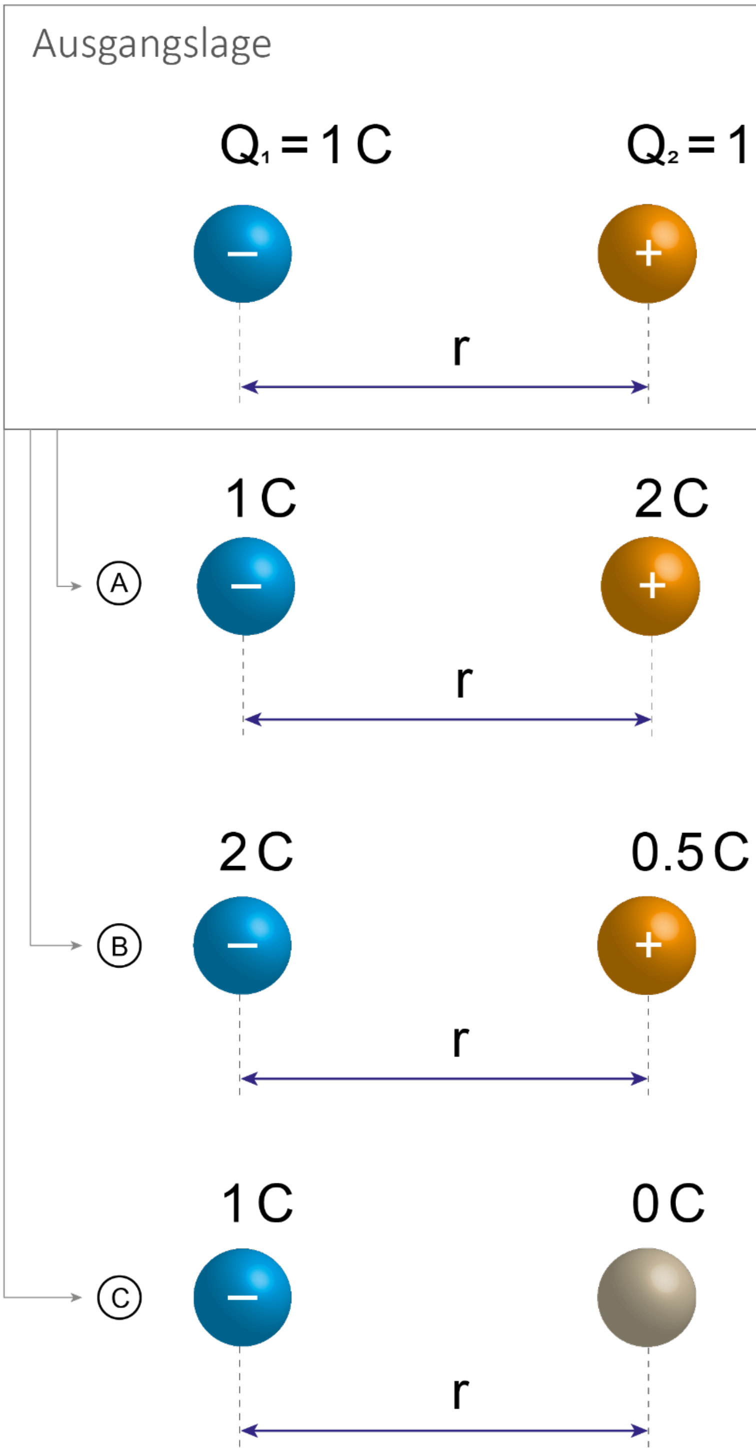
☐ korrekt ☐ falsch Die Kraft halbiert sich.

☐ korrekt ☐ falsch Die Kraft verdoppelt sich.

☐ korrekt ☐ falsch Die Kraft verändert sich nicht.

☐ korrekt ☐ falsch Die Kraft wird vervierfacht.

P14 In der untenstehenden Abbildung finden Sie zwei Ladungen Q_1 und Q_2 im Abstand r. Wir halten den **Abstand r zwischen den Ladungen konstant**, während die **Grösse der Ladungen verändert wird**. Vergleichen Sie jeweils den Ausgangszustand mit den verschiedenen Fällen (A bis C) und kreuzen Sie an, welche Auswirkungen dies auf die Coulombkraft F hat.



Fall A:

☐ korrekt ☐ falsch F wird halbiert.
☐ korrekt ☐ falsch F ändert sich nicht.
☐ korrekt ☐ falsch F wird verdoppelt.
☐ korrekt ☐ falsch F wird vervierfacht.
☐ korrekt ☐ falsch F wirkt nicht mehr (F = 0).

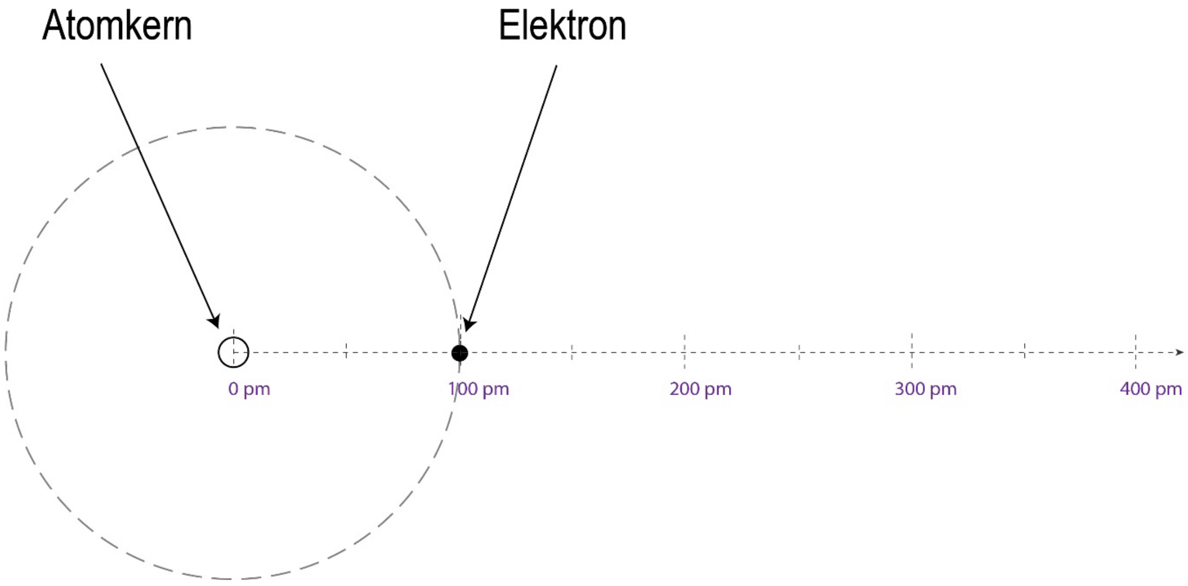
Fall B:

☐ korrekt ☐ falsch F wird halbiert.
☐ korrekt ☐ falsch F ändert sich nicht.
☐ korrekt ☐ falsch F wird verdoppelt.
☐ korrekt ☐ falsch F wird vervierfacht.
☐ korrekt ☐ falsch F wirkt nicht mehr (F = 0).

Fall C:

☐ korrekt ☐ falsch F wird halbiert.
☐ korrekt ☐ falsch F ändert sich nicht.
☐ korrekt ☐ falsch F wird verdoppelt.
☐ korrekt ☐ falsch F wird vervierfacht.
☐ korrekt ☐ falsch F wirkt nicht mehr (F = 0).

P15 Wir betrachten ein Atom mit einem positiv geladenen Atomkern und einem negativ geladenen Elektron, das sich in einer Entfernung von 100 pm zum Atomkern befindet. Auf welche Position müsste man das Elektron bewegen, wenn sich die Coulombkraft auf ein Viertel reduzieren soll? Zeichnen Sie die neue Position des Elektrons in die untenstehende Grafik ein und nennen Sie den Zahlenwert des neuen Abstands.



P16/Q6 Natrium und Chlor reagieren zusammen zu Natriumchlorid (NaCl). Welche der folgenden Aussagen treffen zu?

☐ korrekt ☐ falsch Es bilden sich Natriumionen und Chloridionen, welche sich aufgrund der unterschiedlichen Ladungen gegenseitig anziehen.

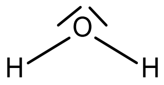
☐ korrekt ☐ falsch Neutrale Natriumatome und neutrale Chloridatome lagern sich in einer gitterartigen Struktur zusammen.

☐ korrekt ☐ falsch Natrium- und Chloratome bilden Elektronenpaarbindungen aus, um Natriumchlorid-Moleküle zu bilden.

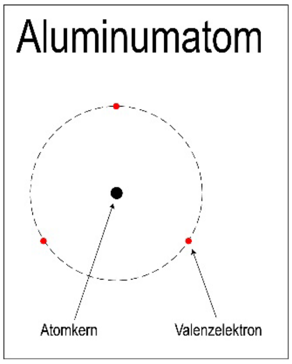
☐ korrekt ☐ falsch Es bilden sich Natriumionen und Chloridionen, welche sich zu Natriumchlorid-Molekülen zusammenschliessen.

☐ korrekt ☐ falsch Jeweils ein Natriumion und ein Chloridion schliessen sich zu einer Einheit zusammen.

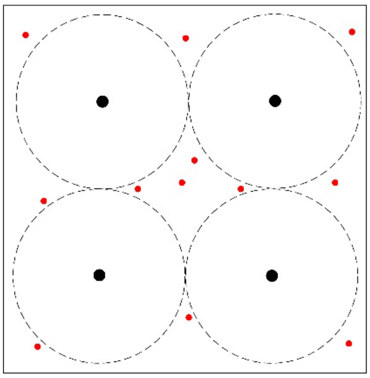
P17 Erläutern Sie, weshalb ein Wassermolekül mit der Molekülformel H_2O nicht spontan in seine Atome zerfällt.



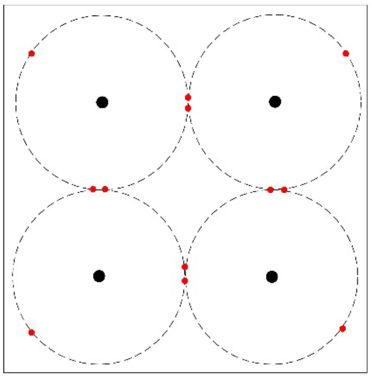
P18/Q20 Nachfolgend ist ein isoliertes Aluminiumatom illustriert. Welche Darstellung illustriert am besten, wie die Atome im gebundenen Zustand vorliegen zum Beispiel in einer Aluminiumfolie.



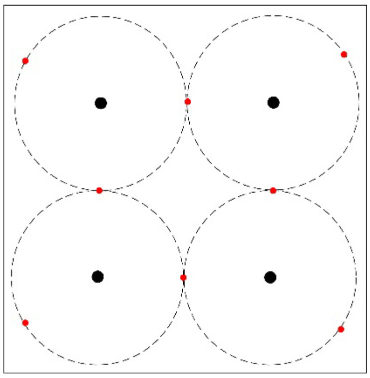
A.

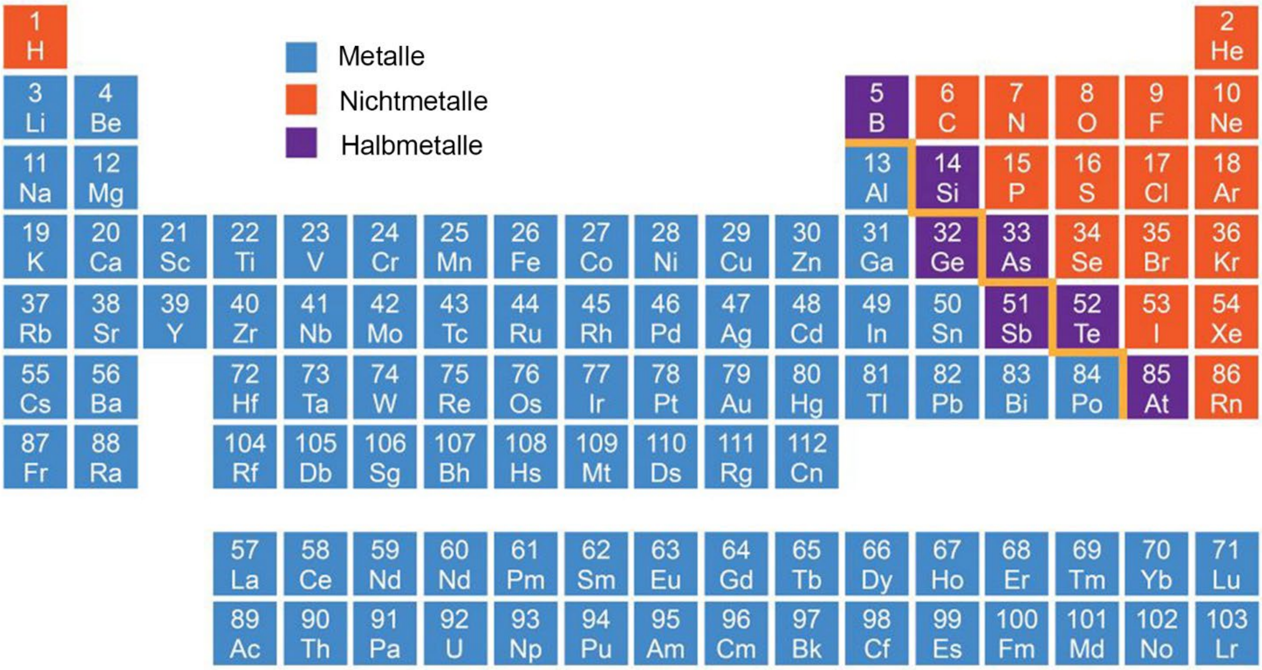


B.



C.





🟦 Metalle
🟧 Nichtmetalle
🟪 Halbmetalle

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn						
			57 La	58 Ce	59 Nd	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
			89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Appendix 1.2: Subscore Assignment

The items of the CBI can be assigned to subscores, as depicted in Table 1.

Table 1: Items with their Subscore Assignment.

		Subscores				
Item	Total score	Ionic	Metallic	Covalent	IMF	Identifying
Q1	1	1				
*Q2**						
Q3	1			1		
Q4	1	1				
Q5	1		1			
Q6	1	1				
Q7	1	1				
Q8.1	1	1				
Q8.2	1	1				
Q9	1			1		
Q10	1			1		
Q11.1	1		1			1
Q11.2	1	1				1
Q11.3	1			1		1
Q11.4	1	1				1
Q12	1		1			
Q13	1	1				
Q14	1		1			
Q15	1		1			
Q16	1			1		
Q17	1				1	
Q18	1				1	
Q19	1	1				
Q20	1		1			
Q21	1			1		
Q22	1					
*Q22.cov**				1		1
*Q22.met**			1			1
*Q22.ionic**		1				1
Q23	1				1	
Q24	2				2	
Q25.1	1			1	1	
Q25.2	1	1	1		1	
Q25.3	1				1	
Total points	**31**	**12**	**8**	**8**	**8**	**7**

Note. * items not included in total score (exclusion or redundancy), IMF = intermolecular forces

Appendix 1.3: Confirmatory Factor Analysis for the CBI

Utilizing university evaluation sample 3 (N = 970), the shown Scree plot indicates that three or four factors would be beneficial for modeling the data (see Figure 1).

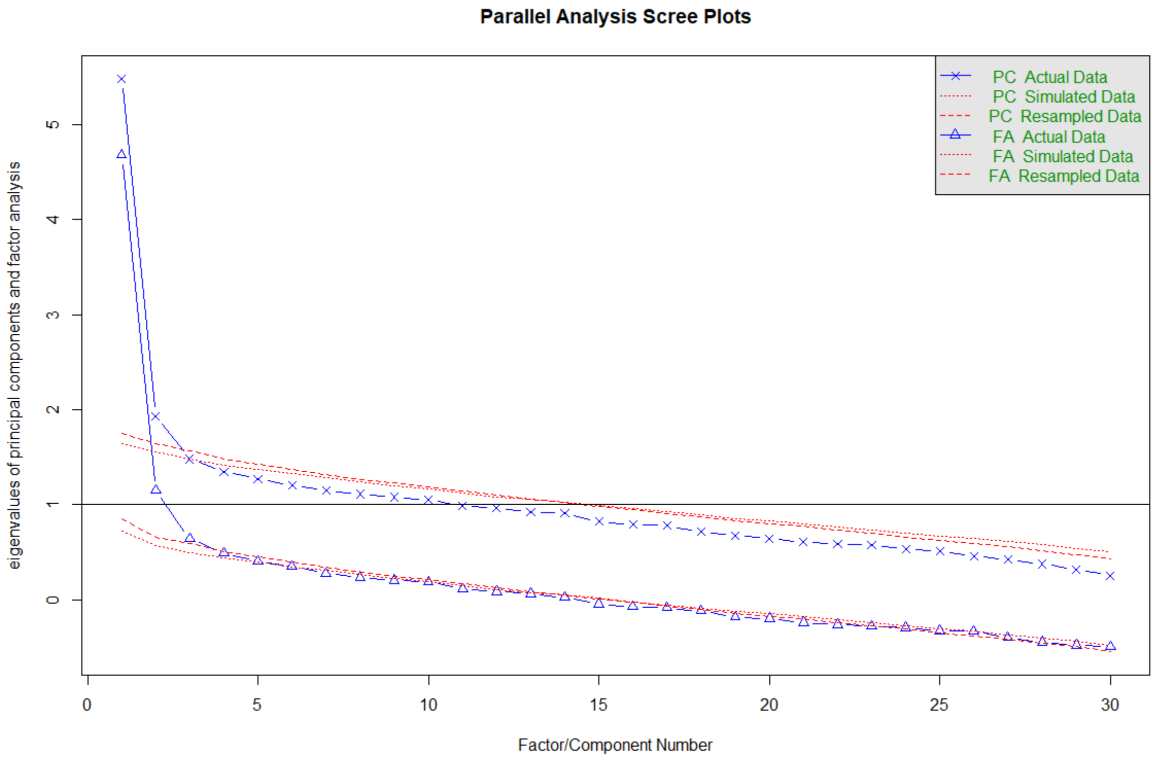


Figure 1: Scree Plot for the results of the chemical bonding inventory administered to university evaluation sample 2 (N = 970)

Appendix 1.4 Subscore Profile Analysis for University Evaluation Sample 2

An investigation into profiles of subscores in the university evaluation sample 2 yielded that students with a lower subscore in one domain will also be low in other subscores. When the data was modeled with one to five subclasses, no crossing of subclasses' subscore values was observed. Modeling the data with 6 subclasses yields the first crossover (see Figure 2). The overall interpretation of the initial profile analysis of subscores is that the subscores are part of the overarching topic of chemical bonding and are hence connected and correlated strongly.

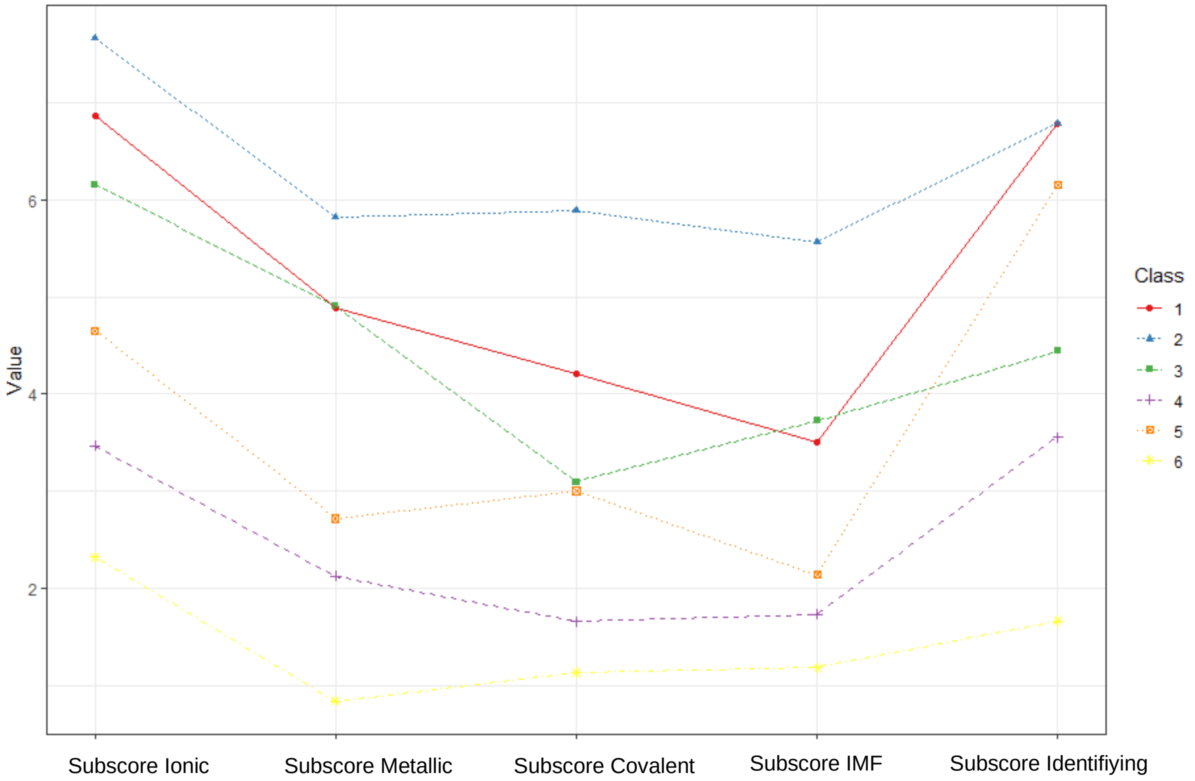


Figure 2: Profile Analysis with 6 profiles showing the first crossing of lines.

Appendix 1.5: CBI pre-test

The chemical bonding inventory pre-test (CBI pre-test) is shown on the following pages.

Appendix 2: Ethics Commission Approval

The Ethics commission approval form is depicted on the following pages

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Vice President for Research

ETH Zurich
Prof. Dr. Detlef Günther
HG F 57
Rämistrasse 101
8092 Zurich

Contact:
Office of Research
ethics@sl.ethz.ch

ETH Zürich
Herr Adrian Zwyssig
Empirische Lehr- und Lernforschung
RZ E 9
Clausiusstrasse 59
8092 Zürich

Zurich, 17 August 2021 PE

EK 2021-N-123: Diagnose und Förderung des Verständnisses der chemischen Bindungslehre

Dear Mr Zwyssig,

Your above proposal, submitted on 22 July 2021, has been reviewed by the following members of the ETH Zurich Ethics Commission:

Prof. Dr. Lutz Wingert, Präsident	Professur für Philosophie
Prof. Dr. Jörg Goldhahn	Institut für Translationale Medizin
Dr. Julian Mausbach	Rechtswissenschaftliches Institut

Based on the Commission's recommendation, the Vice President for Research of ETH Zurich has come to the following decision:

☒ **Approval without reservation** ☐ Approval with reservation ☐ Revise and reply
☐ Revise and resubmit ☐ Rejection ☐ Not evaluated

Final provisions

You are required to inform the Ethics Commission immediately on any of the following occasions:

a) if an event occurred that affects the integrity of the participants or the continuation of the research project;

b) if you wish to make changes to the research protocol or to extend the project; or

c) if the study is prematurely terminated.

Kind regards,

Prof. Detlef Günther
Vice President for Research

Prof. Lutz Wingert
Chair ETH Zurich Ethics Commission

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Gesuch an die Ethikkommission der ETH Zürich

Einzureichen auf www.etappo.ethz.ch

A. Allgemeine Informationen

Projekttitel

Diagnose und Förderung des Verständnisses der chemischen Bindungslehre

Projektleiter/in

Name	Titel	Gruppe / Professur / Institut	Hochschule
Adrian Zwyssig	MSc. ETHZ	Gruppe von Prof. Dr. Elsbeth Stern / Professur für Lehr- und Lernforschung / Institut für Verhaltenswissenschaften Gruppe von Prof. Dr. Antonio Togni / Professur für Metallorganische Chemie/ Labor für anorganische Chemie	ETH Zürich
Elsbeth Stern	Prof. Dr.	Gruppe von Elsbeth Stern / Professur für Lehr- und Lernforschung/ Institut für Verhaltenswissenschaften	ETH Zürich

Beteiligte Mitarbeiter/innen

Name	Titel	Gruppe / Professur / Institut	Hochschule
Antonio Togni	Prof. Dr.	Gruppe von Prof. Dr. Antonio Togni / Professur für Metallorganische Chemie/ Labor für anorganische Chemie	ETH Zürich

Anzahl Probanden/innen	***Dauer der Studie***	***Art des Projektes***
Schulstudie: Minimum: 150 Maximum: 200	Beginn: Oktober 2021 Ende: Dezember 2022	☒ Forschungsprojekt ☐ Projekt Lehre (Masterarbeit)
ETH-Studie: Minimum: 60 Maximum: 100		

1. Abstract

Übergeneralisierung ist eine der grossen Herausforderungen beim Lehren und Lernen neuer naturwissenschaftlicher Konzepte. Eine solche Übergeneralisierung der Lernenden beobachtet man auch bei der chemischen Bindungslehre, eines der wichtigsten Themen im gymnasialen Chemieunterricht. Typischerweise vernachlässigen Lernende den Unterschied zwischen den drei verschiedenen Bindungstypen (kovalente, ionische und metallische Bindungen) und benutzen das Konzept der kovalenten Bindung auch für metallische und ionische Stoffe. Unsere Voruntersuchung mit Studienanfängern an der ETH Zürich (naturwissenschaftliche Fachrichtung, September 2020, N = 1030) hat ergeben, dass diese und weitere verwandte Fehlvorstellungen zur chemischen Bindungslehre verbreitet sind, obwohl die Themen im gymnasialen Chemieunterricht behandelt wurden. Zudem zeigte sich, dass das Unterscheiden von zwischenmolekularen Kräften und chemischen Bindungen vielen Studierenden weiterhin Mühe bereitet. Es drängt sich folglich die Frage auf: Wie lässt sich das Verständnis der chemischen Bindungslehre besser fördern?

Um Verwechslungen und der Übergeneralisierung von ähnlichen Konzepten entgegenzuwirken, haben sich in der Lehr- und Lernforschung vergleichende und kontrastierende Aktivitäten als besonders effektiv erwiesen. Aus diesem Grund habe ich neue Lernmaterialien entwickelt, die viele vergleichende und kontrastierende Aufträge zu den verschiedenen Bindungstypen enthalten, um die Unterschiede zwischen den Bindungstypen besser hervorzuheben. In der Vor- und Nachtest-Untersuchung an Schweizer Gymnasien (N = ca. 200) wird die Experimentalgruppe einer Vergleichsgruppe gegenübergestellt. In der Experimentalgruppe wird untersucht, ob die neu entwickelten Lernmaterialien zu konzeptuellem Wandel führt und das Verständnis der Unterschiede zwischen den verschiedenen Bindungstypen effizient gefördert wird. Dieser Gruppe wird eine Vergleichsgruppe gegenübergestellt, mithilfe derer festgestellt werden soll, wie gross der Lernzuwachs typischerweise bei herkömmlichem Unterricht zur Bindungslehre ist. Zusätzlich wird eine Kurzversion der Unterrichtseinheit angehenden ETH Studierenden vermittelt und untersucht, ob diese Kurzintervention zu einem Lernzuwachs führt.

2. Projektbeschrieb

Das Projekt besteht aus einer ausgedehnten Untersuchung an Schweizer Gymnasien (siehe 2.4.2) und einer kleineren Untersuchung mit angehenden ETH Studierenden, deren Studium die Vorlesung «Allgemeine Chemie» in ihrem Grundstudium enthält (siehe 2.4.3).

2.1 Zielsetzung der Projekte

Die Zielsetzung des Projekts ist es, Verständnisschwierigkeiten beim Konzept der chemischen Bindungslehre zu identifizieren sowie die neu entwickelte Unterrichtseinheit zum Thema der chemischen Bindungslehre auf der Gymnasialstufe auf deren Effizienz bei der Förderung des Verständnisses zu untersuchen. Zusätzlich wird eine Kurzform angehenden ETH Studierenden präsentiert und evaluiert, ob eine solche Kurzintervention zu einem verbesserten Verständnis der chemischen Bindungslehre beiträgt.

2.2 Ergebnisse der Voruntersuchung

Um herauszufinden, welche Aspekte beim Verständnis der chemischen Bindungslehre besonders schwer zu erfassen sind, wurde im September 2020 eine Voruntersuchung mit 1030 Erstsemestrigen an der ETH Zürich vorgenommen. Diese Untersuchung wurde im Rahmen der regulären Vorlesungen durchgeführt und ersetzte einen anderen Fragebogen, der ansonsten verwendet wurde, um das Vorwissen der Studierenden zu erfassen. Dabei wurde das Konzeptverständnis im Bezug auf die chemische Bindungslehre der Erstsemestrigen der folgenden Vorlesungen geprüft:

- «Allgemeine Chemie I» (529-0011-02L)	Dozent: Prof. Dr. Antonio Togni
- «Allgemeine Chemie» (für Biol./Pharm.Wiss., 529-1001-01L)	Dozent: Dr. Jan Cvengros
- «Allgemeine Chemie» (für HST, 529-1001-03L)	Dozent: Dr. Jan Cvengros

Die Untersuchung wurde in der zweiten Woche des Herbstsemesters 2020 im Rahmen der Übungsstunden der regulären Vorlesungen durchgeführt. Die in den Übungsstunden anwesenden Studierenden füllten dabei an ihren eigenen Laptops die anonyme Onlineumfrage durch. Die Durchführung fand in Absprache und unter Supervision der Dozierenden statt und wurde im Rahmen der Lehre und Optimierung der Vorlesungen vorgenommen. Die Teilnehmenden hatten dabei die Option anzuklicken, dass ihre Daten nicht zu wissenschaftlichen Zwecken verwendet werden dürfen. Ausser dem Jahrgang, Geschlecht und Studiengang wurden keine weiteren persönlichen Daten erfasst, was eine Rückführung auf einzelne Studierenden verhinderte. Auf die Erfassung von Namen oder der ETH-Matrikelnummer wurde explizit verzichtet, womit die Anonymisierung gewährleistet werden konnte. Damit die Studierenden einen Einblick in ihre eigenen Resultate erhalten konnten, wurde ein rein zufälliger Code erzeugt, der es den Studierenden erlaubte, ihre eigenen Resultate später einzusehen. Nach der Auswertung wurde in der regulären Vorlesung auf typische Misskonzepte und Verständnisschwierigkeiten eingegangen.

Die Auswertung der ausgefüllten Online-Fragebögen bestätigte die Vermutung, dass ein Teil der Lernenden den Unterschied zwischen den drei verschiedenen Bindungstypen (kovalente, ionische und metallische Bindungen) typischerweise vernachlässigt und das Konzept der kovalenten Bindung auch für metallische und ionische Stoffe verwendet. Es zeigte sich, dass diese und weitere Fehlvorstellungen zur chemischen Bindungslehre verbreitet sind, obwohl die Themen im gymnasialen Chemieunterricht behandelt wurden. Zudem konnte festgestellt werden, dass das Unterscheiden von zwischenmolekularen Kräften von chemischen Bindungen vielen Studierenden weiterhin Mühe bereitet. Es drängte sich folglich die Frage auf: Wie lässt sich das Verständnis der chemischen Bindungslehre besser fördern? Dies motivierte die Erstellung einer Unterrichtseinheit, die stärker auf die festgestellten Schwierigkeiten eingeht.

2.3 Arbeitsplan und zeitlicher Ablauf

2019	Erstellung des Fragebogens zur Diagnose des Verständnisses der chemischen Bindungslehre (abgeschlossen)
2020	Diagnose des Verständnisses der chemischen Bindungslehre bei Erstsemestrigen an der ETH Zürich (abgeschlossen)
2019 – 2021	Erstellung und Optimierung der Unterrichtseinheit zur chemischen Bindungslehre
2021 – 2022	Evaluierung der Unterrichtseinheit zur chemischen Bindungslehre in einer Vor- und Nachtest-Untersuchung an Schweizer Gymnasien
Herbstsemester 2021	Erprobung der Kurzform der Unterrichtseinheit mit angehenden ETH Studierenden
Herbstsemester 2022	Allfällige Wiederholung des Unterrichts mit der Kurzform der Unterrichtseinheit mit angehenden ETH Studierenden.

2.4 Untersuchungsmethoden

2.4.1 Entwicklung einer neuen Unterrichtseinheit

Um Verwechslungen und der Übergeneralisierung von ähnlichen Konzepten entgegenzuwirken, haben sich in der Lehr- und Lernforschung vergleichende und kontrastierende Aktivitäten als besonders effektiv erwiesen. Aus diesem Grund habe ich neue Lernmaterialien entwickelt, die viele vergleichende und kontrastierende Aufträge zu den verschiedenen Bindungstypen enthalten, um die Unterschiede zwischen den Bindungstypen besser hervorzuheben.

Um zu garantieren, dass die entwickelte Unterrichtseinheit den Lernenden für den weiteren Verlauf des Chemieunterrichts keinen Nachteil verschafft, wurde die Unterrichtseinheit in Zusammenarbeit mit einer pensionierten Gymnasiallehrperson entwickelt, die eine Unterrichtserfahrung von 35 Jahren aufweist und für das MINT-Lernzentrum bereits mehrere optimierte Unterrichtseinheiten erstellt hat. Der Studienleiter hat die neu entwickelte Unterrichtseinheit anschliessend zweimal (Start Dezember 2019 und Oktober 2020) in Zusammenarbeit mit erfahrenen Praxislehrpersonen, die in der didaktischen Ausbildung angehender Chemielehrpersonen engagiert sind, angewandt und weiter optimiert. Die Unterrichtseinheit wurde von Chemielehrpersonen als ausgereift und als spannende Möglichkeit aufgefasst, das Thema der chemischen Bindungslehre zu unterrichten.

Nach erfolgreicher Pilotierung der Version für das Gymnasium wird eine verkürzte Form erarbeitet, die sich an angehende ETH Studierende richtet. Dabei ist zu beachten, dass diese Lernenden in gymnasialen Chemieunterricht das Thema bereits behandelt haben. Aufbauend aus den Erfahrungen der Voruntersuchung können wir verstärkt auf noch bestehende Verständnisschwierigkeiten eingehen.

2.4.2 Interventionsstudie an Schweizer Gymnasien

In der geplanten Interventionsstudie an Schweizer Gymnasien (N = ca. 200) wird die Experimentalgruppe einer Vergleichsgruppe gegenübergestellt. In der Experimentalgruppe wird untersucht, ob die neu entwickelten Lernmaterialien zu konzeptuellem Wandel führen und ob das Verständnis der Unterschiede zwischen den verschiedenen Bindungstypen effizient gefördert wird. Dieser Gruppe wird eine Vergleichsgruppe gegenübergestellt, mithilfe derer festgestellt werden soll, wie gross der Lernzuwachs typischerweise bei herkömmlichen Unterricht zur Bindungslehre ist. Das Studiendesign ist in Abb. 1 dargestellt.

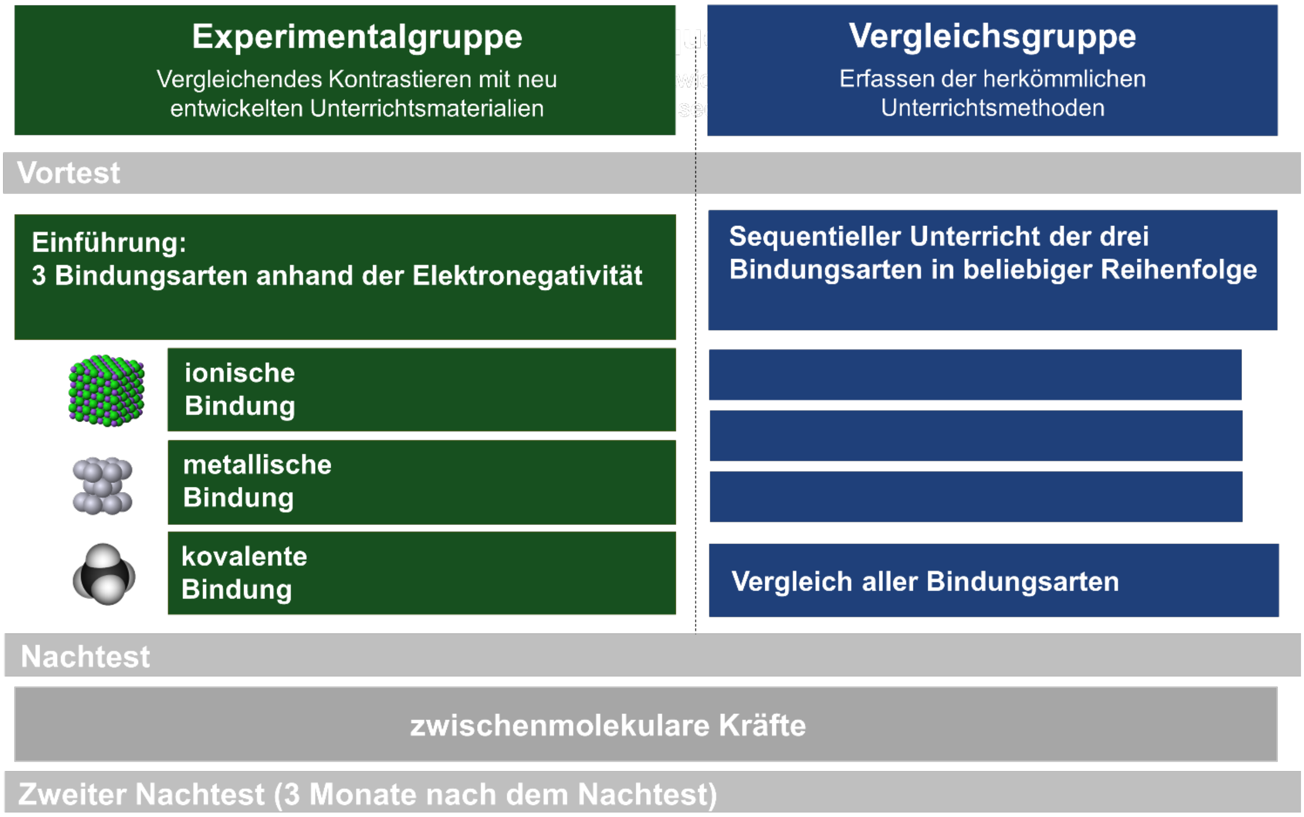


Abb. 1: Darstellung des Studiendesigns an Schweizer Gymnasien: Die Lehrperson unterrichtet jeweils die eine Parallelklasse mit den neu entwickelten Unterrichtsmaterialien (Experimentalgruppe), während die andere Parallelklasse den herkömmlichen Unterricht erhält (Vergleichsgruppe). Es werden zu drei Zeitpunkten Tests zum Erfassen des Verständnisses der chemischen Bindungslehre durchgeführt.

Vortest

Der Vortest besteht aus 15 Fragestellungen im Multiple-Choice-Format sowie drei Fragestellungen im offenen Format. Die Fragen befassen sich mit Konzepten, die für das Verständnis der chemischen Bindungslehre von Bedeutung sind. Dieser Test wird vor dem Unterricht zur Bindungslehre durchgeführt. Beispielsaufgaben sind unter Anhang 8.2 einsehbar.

Nachtest

Der Nachtest besteht aus 22 Fragestellungen im Multiple-Choice-Format, die das Verständnis der chemischen Bindungslehre untersuchen und folgt dem vollständigen Vermitteln der drei Bindungsarten. Dieser Fragebogen entspricht in grossen Teilen dem Online-Fragebogen, der von den Erstsemestrigen an der ETH Zürich ausgefüllt wurde. Beispielsaufgaben sind unter Anhang 8.3 einsehbar.

Zweiter Nachtest

Der Nachtest wird drei Monate nach dem Nachtest wiederholt und untersucht mögliche Langzeiteffekte bei der Experimental- und Vergleichsgruppe. Dieser Test enthält noch drei zusätzliche Fragen zu den zwischenmolekularen Kräften.

Subtest zu kognitiven Fähigkeiten und sozioökonomischer Status

Um sicherzustellen, dass die Vergleichbarkeit der verschiedenen Schulklassen gegeben ist, wird zusätzlich ein Subtest zu den kognitiven Fähigkeiten eingesetzt: Kognitiver Fähigkeitstest für die 10. Klasse (Heller und Perleth 2000). Es wird explizit auf die Berechnung eines Intelligenzquotienten verzichtet und ausschliesslich mit Rohwerten gerechnet. Dieser Test ist ein standardisierter Test, der bereits vielfach zu Forschungszwecken eingesetzt wurde. Zusätzlich wird ein Fragebogen ausgeteilt, der den sozioökonomischen Status der Lernenden abbilden soll. Beispiele sind im Anhang 8.4 und 8.5 einsehbar. Diese zwei Tests werden in einer vergleichbaren, von der Ethik-Kommission bewilligten Untersuchung bereits eingesetzt (TraM-Studie/Swiss-MINT-Study).

Quelle: Heller, Kurt & Perleth, Christoph. (2000). Kognitiver Fähigkeitstest für 4. bis 12. Klassen, Revision : KFT 4-12+R ; Manual.

2.4.3 Interventionsstudie an der ETH Zürich

Um die Fragestellung zu klären, ob eine kurze Intervention mit einer Fokussierung auf die typischen Verständnisschwierigkeiten zu einem verbesserten Verständnis der chemischen Bindungslehre führt wird eine Untersuchung mit angehenden ETH Studierenden in der Woche vor dem Studienbeginn durchgeführt. Die Rekrutierung geschieht durch Anschrift via E-Mail. Die interessierten ETH Erstsemestrigen werden dann in zwei Gruppen eingeteilt: die Interventionsgruppe und die Vergleichsgruppe. Beide Gruppen erhalten die Kurzform der neu erstellten Unterrichtseinheit, jedoch wird bei der Kontrollgruppe der Vor- und Nachtest vor dem Unterricht durchgeführt, um den Retest-Effekt zu messen. Auf diese Weise entstehen keine Nachteile für die Studienteilnehmenden in der Vergleichsgruppe. Im Rahmen der regulären Vorlesungen wird das Verständnis der chemischen Bindungslehre nochmals via Online-Test bei sämtlichen Erstsemestrigen untersucht (Abb. 2). Auf die Messung der kognitiven Fähigkeiten sowie des sozioökonomischen Status’ wird in dieser Studie verzichtet.

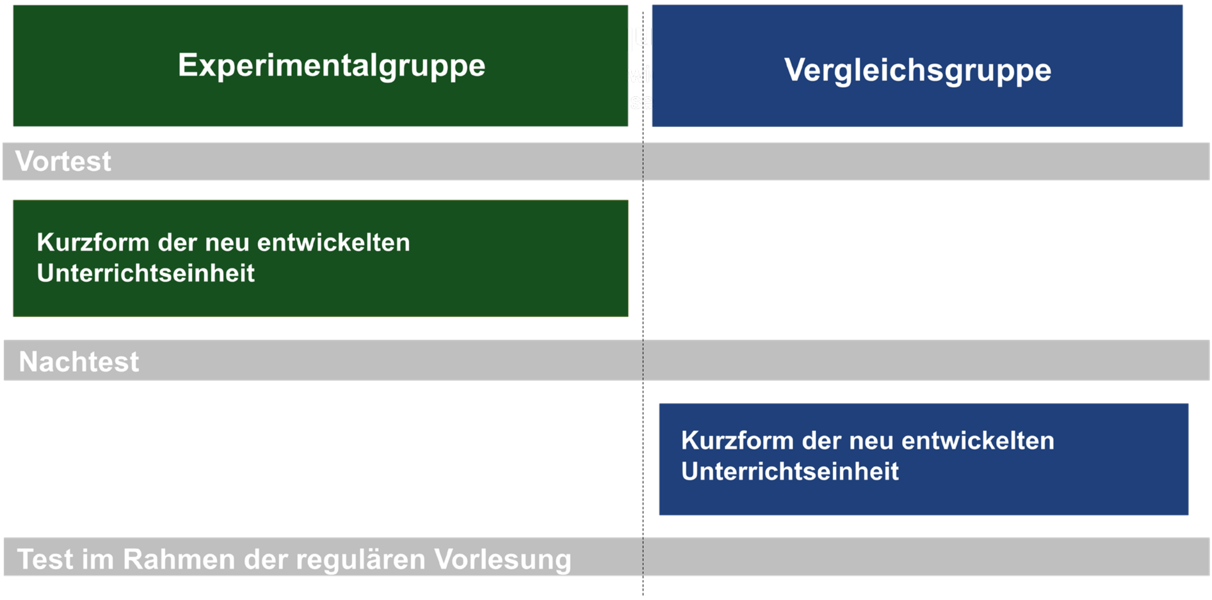


Abb. 2: Darstellung des Wartegruppe-Studiendesigns für die Untersuchung mit angehenden ETH Studierenden.

3. Zu erwartende Risiken und entsprechende Vorsichtsmassnahmen

3.1 Direkte Risiken durch Untersuchung

Da die Untersuchung im regulären Schulalltag stattfinden wird, sind keine Risiken zu erwarten. Die neuen Unterrichtsmaterialien sind sorgfältig entwickelt, ausreichend erprobt und von mehreren erfahrenen Chemielehrpersonen auf deren Anwendbarkeit überprüft worden. Die vermittelten Themen entsprechen Inhalten, die in regulären Lehrplänen Deutschschweizer Gymnasien anzutreffen sind. Da die Vergleichsgruppe den regulären Unterricht der Lehrperson erfährt, ist auch diese Gruppe keinem Risiko ausgesetzt. Die Lehrpersonen erhalten durch die Teilnahme an der Studie eine Weiterbildung und zudem neue Einblicke und neue Impulse für ihren Unterricht.

Die Teilnahme am Kurs für ETH Studierende ist freiwillig und stellt ein Zusatzangebot zu den regulären Vorlesungen dar. Die vermittelten Inhalte sind Teil des gymnasialen Curriculums und werden grösstenteils zu Studienbeginn vorausgesetzt.

3.2 Datensicherheit

3.2.1 Datenerhebung und Anonymisierung

Sämtliche Tests werden ohne Namen der Untersuchungsteilnehmenden durchgeführt. Zu keinem Zeitpunkt werden die Namen der Untersuchungsteilnehmenden und die Ergebnisse zum Verständnis der chemischen Bindungslehre, des Kognitionstests oder zum sozioökonomischen Status gemeinsam erfasst oder abgespeichert.

Die Tests werden auf Papier ausgefüllt und anschliessend in eine Excel-Datentabelle eingetragen und ausschliesslich auf Laufwerken der ETH Zürich gespeichert. Die Tests in Papierform werden abgeschlossen aufbewahrt. Die Bearbeitung und Einsehung der Daten erfolgt ausschliesslich von an der Studie beteiligten Forschenden und Hilfsassistierenden.

3.2.2 Datenlöschung

Die Erstellung eines Codes (siehe Anhang 8.1) erlaubt es den Teilnehmenden, ihre Resultate einzusehen, ohne dass die Lehrperson oder die Studienleitung die Lernenden eindeutig identifizieren könnten. Entsprechend ist die nachträgliche Beantragung der Löschung der Daten weiterhin gewährleistet, ohne zu riskieren, dass sensible Daten gemeinsam mit eindeutigen Identifikationsmerkmalen erfasst und gespeichert werden müssen.

3.3 Reputationsschaden für die ETH Zürich

Da die Unterrichtsmaterialien erfolgreich erprobt und durchgängig auf positive Rückmeldungen bei Lehrpersonen wie auch Lernenden gestossen sind, ist nicht mit einem Reputationsschaden zu rechnen. Im Gegenteil, durch das aktive Engagement für eine mögliche Förderung des Verständnisses eines wichtigen Grundkonzeptes im gymnasialen Chemieunterricht ist eine Steigerung des Ansehens das wahrscheinlichere Szenario. Da sämtliche Daten anonymisiert und ohne Namen an sicheren Orten abgespeichert sind, ist auch nicht mit datentechnischen Problemen zu rechnen.

4. Lebensläufe

Die Lebensläufe und die Publikationslisten der Projektleitung und der Lebenslauf des Projektmitarbeiters sind am Ende des Antrages zu finden (Anhang 8.6).

Projektleitung

Adrian Zwyssig (CV inkl. Publikationsliste)

Prof. Dr. Elsbeth Stern (CV inkl. Publikationsliste)

Projektmitarbeiter

Prof. Dr. Antonio Togni (CV)

5. Probanden/innen

5.1 Interventionsstudie an Schweizer Gymnasien

Die Rekrutierung erfolgt durch das Anschreiben der Praktikumslehrpersonen, die in der didaktischen Ausbildung der Chemielehrpersonen der ETH involviert sind.

Die Anzahl der Schülerinnen und Schüler kann zum jetzigen Zeitpunkt nur ungefähr abgeschätzt werden, da weiterhin interessierte Lehrpersonen rekrutiert werden. Im Moment wird mit einer Teilnahme von ungefähr fünf Lehrpersonen gerechnet. Bei der Annahme von durchschnittlich 20 Schülerinnen und Schülern pro Klasse entspricht das 200 Studienteilnehmenden.

Bedingung für die Teilnahme an der Studie ist das Vorhandensein von Parallelklassen, da dies das Studiendesign vorschreibt. Die Zuteilung der Parallelklassen zur Interventionsgruppe oder Vergleichsgruppe wird nach dem Zufallsprinzip festgelegt.

5.2 Interventionsstudie an der ETH

Die Rekrutierung erfolgt über den Versand eines E-Mails mit dem Angebot des Kurzkurses. Das Schreiben richtet sich an alle Interessierten der angehenden ETH Studierenden, deren Studium die Vorlesung «Allgemeine Chemie» in ihrem Grundstudium enthält.

Die genaue Anzahl der Teilnehmenden steht noch nicht fest. Es wird mit einer maximalen Teilnehmerzahl von 100 Studierenden gerechnet.

6. Informationsblatt für Probanden/innen

Siehe Beilage 6.

7. Einverständniserklärung

Siehe Beilage 7.

Beilage 6: Informationsblatt für Dateneigner

Titel der Studie: Diagnose und Förderung des Verständnisses der chemischen Bindungslehre

a) Zielsetzung der Studie	Untersuchungen mit Studienanfängerinnen und Studienanfängern an der ETH Zürich haben ergeben, dass das zentrale Konzept der chemischen Bindungen nur unzureichend im Schulunterricht verstanden wurde. Mit dieser Studie möchten wir herausfinden, ob der Einsatz neu entwickelter Unterrichtsmaterialien zur chemischen Bindungslehre zu einem besseren Verständnis führt. Wir möchten detailliert untersuchen, welche Vorteile der neue Ansatz im Vergleich zu herkömmlichem Unterricht hat. Wenn die Erprobung erfolgreich ist, sollen in einer nächsten Phase die Unterrichtsmaterialien weiteren Lehrpersonen zur Verfügung gestellt werden, damit weitere Schülerinnen und Schüler von den gewonnenen Erkenntnissen profitieren können.
b) Untersuchungen	Wir untersuchen, ob die neu entwickelten Unterrichtsmaterialien zu einem besseren Verständnis der chemischen Bindungslehre beitragen. Dazu werden zu verschiedenen Zeitpunkten Tests durchgeführt, einige zusätzliche Daten erhoben und den Lehrpersonen die notwendigen Unterrichtsmaterialien zur Verfügung gestellt. Um zu kontrollieren, ob die verschiedenen teilnehmenden Klassen miteinander vergleichbar sind, wird zudem die Kurzversion eines Tests zum schlussfolgernden Denken vorgelegt. Dieser Test kann nicht zur Berechnung des Intelligenzquotienten (IQ) verwendet werden und wird, wie sämtliche Tests, komplett anonym durchgeführt. Die individuellen Ergebnisse der verschiedenen Tests sind für Lehrpersonen zu keinem Zeitpunkt einsehbar und haben damit auch keinen Einfluss auf die Notengebung an der Kantonsschule.
c) Ablauf	Vor und nach dem Unterricht zur chemischen Bindungslehre wird ein anonymer Test durchgeführt, um die Lernzuwächse zu erfassen. Drei Monate nach dem Beenden der Unterrichtseinheit wird nochmals ein Test durchgeführt, um mögliche Langzeiteffekte festzustellen.
d) Bedingungen für die Studienteilnahme	Es werden Klassen von Lang- und Kurzzeitgymnasien der Deutschschweiz untersucht, die das Thema der chemischen Bindungslehre noch nicht behandelt haben.
e) Vor- und Nachteile für StudienteilnehmerInnen / Risiken	Die Studienteilnahme birgt keinerlei Risiken oder Nachteile. Der Vorteil liegt darin, dass unsere Forschung langfristig dazu dienen kann, neue Ansätze für den Chemieunterricht am Gymnasium zu liefern.
f) Finanzierung	Das Projekt wird vollständig durch Forschungsmittel der ETH Zürich finanziert (Lehrstuhl für empirische Lehr- und Lernforschung sowie Professur für Metallorganische Chemie).
g) Entschädigung	Für die Teilnahme an der Studie erhält jede Klasse 200 CHF in ihre Klassenkasse.
h) Rücktrittsrecht	Sie können Ihre Mitwirkung an der Studie jederzeit ohne Angabe von Gründen beenden, ohne dass Ihnen daraus Nachteile entstehen. Auch Eltern können die Teilnahme ihrer Kinder jederzeit ohne Nachteile beenden.

i) Datenschutz	Alle erhobenen Daten werden schon bei ihrer Eingabe anonymisiert, d.h. ohne Namen erfasst. In unseren Veröffentlichungen nennen wir keine Namen oder Adressen, sodass keine Rückschlüsse auf die Person möglich sind. Weder Ihre Lehrpersonen oder Eltern erfahren die persönlichen Ergebnisse. Die zuständigen Untersuchenden und Mitglieder der Ethikkommission der ETH Zürich können die Originaldaten zu Prüf- und Kontrollzwecken einsehen, jedoch unter strikter Einhaltung der Vertraulichkeit.
j) Versicherungsschutz	Allfällige Gesundheitsschäden, die in direktem Zusammenhang mit der Studie entstehen und auf nachweisliches Verschulden der ETH Zürich zurückzuführen sind, sind durch die Betriebs-Haftpflichtversicherung der ETH Zürich (Police Nr. 30/4.078.362, Basler Versicherung AG) gedeckt. Darüber hinaus liegt die Unfall-/Krankenversicherung (z.B. für die Hin- und Rückreise) in der Verantwortung der Probandin/des Probanden.
k) Kontaktpersonen	Bei Fragen oder Unklarheiten kann jederzeit der Studienleiter kontaktiert werden. Adrian Zwyssig adrian.zwyssig@gess.ethz.ch +41 44 633 84 39

Beilage 7: Einverständniserklärung für Schüler/innen

⇒ Bitte lesen Sie dieses Formular sorgfältig durch.
⇒ Bitte fragen Sie den/die Untersucher/in oder Ihre Kontaktperson, wenn Sie etwas nicht verstehen oder etwas wissen möchten.

Titel der Studie: Diagnose und Förderung des Verständnisses der chemischen Bindungslehre

Durchführungsort der Studie: in den Schulräumen der teilnehmenden Gymnasien

Untersucher/in: Adrian Zwyssig (adrian.zwyssig@gess.ethz.ch)

Schüler/in (Name und Vorname):

⇒ Ich nehme an dieser Studie freiwillig teil und kann jederzeit ohne Angabe von Gründen meine Zustimmung zur Teilnahme widerrufen, ohne dass mir deswegen Nachteile entstehen.
⇒ Ich wurde mündlich und/oder schriftlich über die Ziele und den Ablauf der Studie informiert.
⇒ Ich habe die schriftliche Information zur Studie gelesen. Meine Fragen im Zusammenhang mit der Teilnahme an dieser Studie sind mir zufriedenstellend beantwortet worden.
⇒ Ich hatte genügend Zeit, um meine Entscheidung zu treffen.
⇒ Ich bin darüber informiert, dass die allgemeine Betriebs-Haftpflichtversicherung der ETH Zürich (Police Nr. 30/4.078.362, Basler Versicherung AG) nur Gesundheitsschäden deckt, die in direktem Zusammenhang mit der Studie entstehen und auf nachweisliches Verschulden der ETH Zürich zurückzuführen sind. Darüber hinaus liegt die Unfall-/Krankenversicherung (z.B. für die Hin- und Rückreise) in meiner Verantwortung.
⇒ Ich bin einverstanden, dass die zuständigen Untersuchenden und/oder Mitglieder der Ethikkommission zu Prüf- und Kontrollzwecken meine Originaldaten einsehen dürfen, jedoch unter strikter Einhaltung der Vertraulichkeit.

Ort, Datum . . . . Unterschrift Schüler/in . . . .

Ort, Datum . . . . Unterschrift Untersucher/in . . . .

8. Anhang

8.1 Erstellung des persönlichen Codes zur späteren Rückverfolgung oder Datenlöschung

Wichtige Hinweise:
Der Fragebogen wird **ohne Namen und anonym erhoben.** Damit eine Zuweisung von Vortest zum Nachtest möglich ist, müssen Sie jedoch zweimal den gleichen Code generieren.

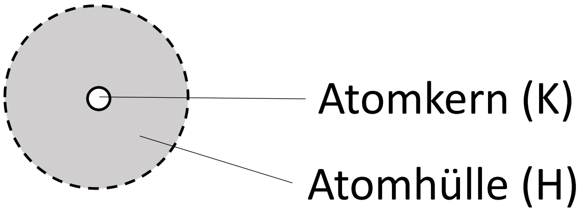
Persönlicher Code:

(1)	(2)	(3)	(4)	(5)

(1) Anfangsbuchstabe des Vornamens Ihrer Mutter *(z. B.* ***N****ina = N)*
(2) Ihr Geburtsmonat als **zweistellige** Zahl *(z. B. Oktober = 10)*
(3) Letzter Buchstabe des Vornamens Ihres Vaters (*z.B. Herber****t*** *= T*)
(4) Ihr Jahrgang als zweistellige Zahl (*z.B. 2004 = 04*)
(5) Ihr Geschlecht *(****W*** *für weiblich,* ***M*** *für männlich, D für Divers)*

8.2 Beispielaufgaben Vortest

1. Die Abbildung illustriert ein Atom mit Atomkern (K) und Atomhülle (H).



a. Im Atomkern (K) befinden sich typischerweise folgende Elementarteilchen:

☐ korrekt ☐ falsch Elektronen

☐ korrekt ☐ falsch Protonen

☐ korrekt ☐ falsch Neutronen

☐ korrekt ☐ falsch Ionen

7. Unter der ersten Ionisierungsenergie eines Atoms versteht man die Energie, die aufgewendet werden muss, …

☐ korrekt ☐ falsch … um der Elektronenhülle eines Atoms ein Elektron zu entfernen.

☐ korrekt ☐ falsch … um der Elektronenhülle eines Atoms ein zusätzliches Elektron hinzuzufügen.

☐ korrekt ☐ falsch … um ein Atom in ein Ion mit positiver oder negativer Ladung umzuwandeln.

☐ korrekt ☐ falsch … um ein Atom in ein positiv geladenes Ion umzuwandeln.

8.3 Beispielaufgaben Nachtest

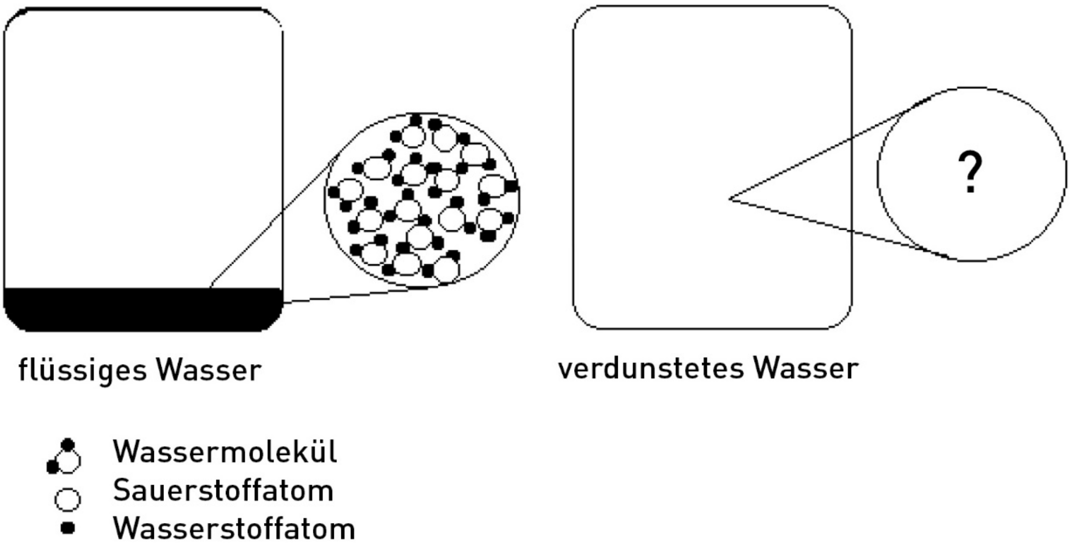
1. Wir betrachten einen Salzkristall (NaCl). In welcher Weise liegen Natrium und Chlor in dieser Verbindung vor?

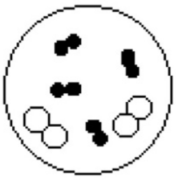
☐ korrekt ☐ falsch als neutrale Natriumatome und neutrale Chloratome

☐ korrekt ☐ falsch als Natrium-Chlorid-Moleküle

☐ korrekt ☐ falsch als Natriumionen und Chloridionen

23. Der Kreis auf der linken Seite zeigt eine vergrösserte Ansicht einer ganz kleinen Menge flüssigen Wassers in einem geschlossenen Gefäss. Was würde die vergrösserte Ansicht zeigen, nachdem das Wasser verdunstet ist? Wählen Sie eine der unten aufgeführten Optionen aus.

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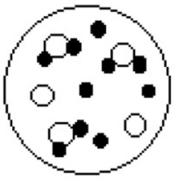
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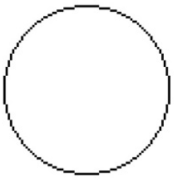
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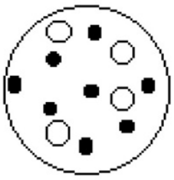
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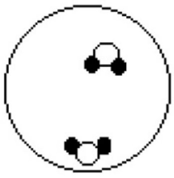
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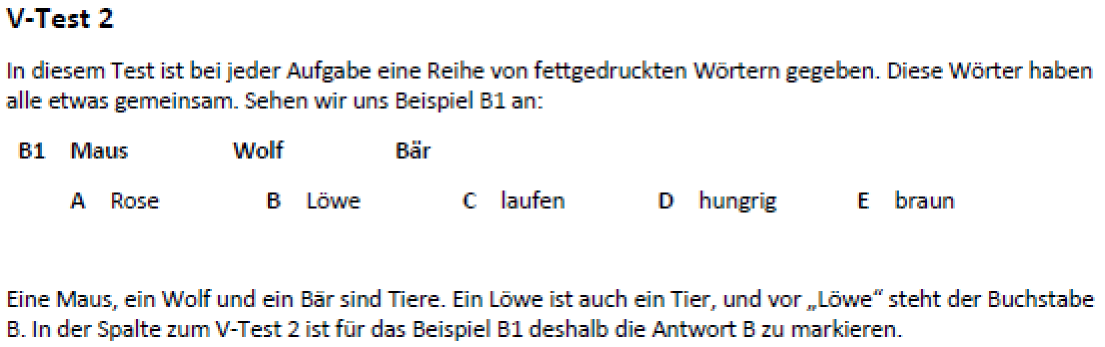
8.4 Beispielaufgaben aus dem KFT 10 - Subtest für die Messung der kognitiven Fähigkeiten



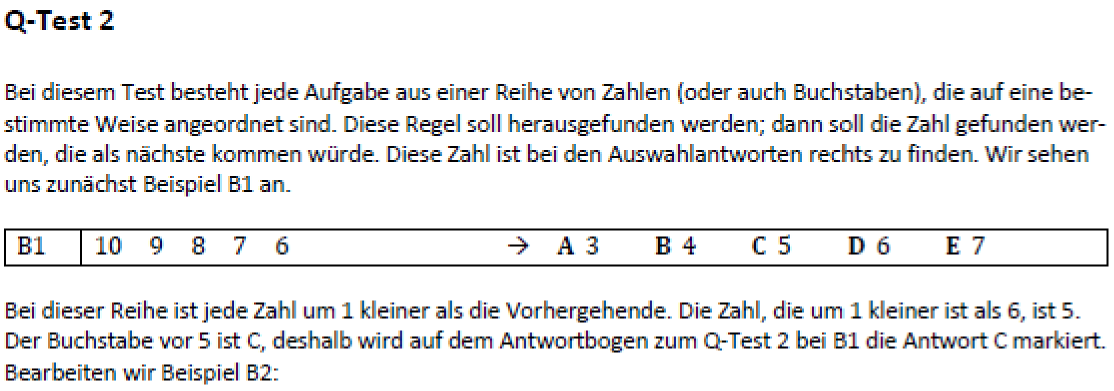
V-Test 2

In diesem Test ist bei jeder Aufgabe eine Reihe von fettgedruckten Wörtern gegeben. Diese Wörter haben alle etwas gemeinsam. Sehen wir uns Beispiel B1 an:

B1 Maus Wolf Bär

A Rose B Löwe C laufen D hungrig E braun

Eine Maus, ein Wolf und ein Bär sind Tiere. Ein Löwe ist auch ein Tier, und vor „Löwe" steht der Buchstabe B. In der Spalte zum V-Test 2 ist für das Beispiel B1 deshalb die Antwort B zu markieren.



Q-Test 2

Bei diesem Test besteht jede Aufgabe aus einer Reihe von Zahlen (oder auch Buchstaben), die auf eine bestimmte Weise angeordnet sind. Diese Regel soll herausgefunden werden; dann soll die Zahl gefunden werden, die als nächste kommen würde. Diese Zahl ist bei den Auswahlantworten rechts zu finden. Wir sehen uns zunächst Beispiel B1 an.

B1	10 9 8 7 6 → **A** 3 **B** 4 **C** 5 **D** 6 **E** 7

Bei dieser Reihe ist jede Zahl um 1 kleiner als die Vorhergehende. Die Zahl, die um 1 kleiner ist als 6, ist 5. Der Buchstabe vor 5 ist C, deshalb wird auf dem Antwortbogen zum Q-Test 2 bei B1 die Antwort C markiert. Bearbeiten wir Beispiel B2:

8.5 Fragen für die Erfassung des sozioökonomischen Status'

Im Folgenden sind die Testfragen zur Erfassung des sozioökonomischen Status' aufgeführt.

1. Ist Ihre erziehungsberechtigte Person alleinerziehend? ☐ **nein** ☐ **ja**

2. a) In welchem Land wurden Sie und Ihre Eltern/Erziehungsberechtigten geboren?

	Ihr Vater bzw. Ihre männliche Bezugsperson (z.B. Stief- oder Pflegevater)	Ihre Mutter bzw. Ihre weibliche Bezugsperson (z.B. Stief- oder Pflegemutter)	Sie
Schweiz, Liechtenstein	☐	☐	☐
Deutschland, Österreich	☐	☐	☐
Frankreich, Belgien	☐	☐	☐
Italien	☐	☐	☐
Spanien	☐	☐	☐
Portugal	☐	☐	☐
Bosnien, Kroatien, Mazedonien, Montenegro, Serbien, Slowenien	☐	☐	☐
Albanien, Kosovo	☐	☐	☐
Türkei	☐	☐	☐
Skandinavien	☐	☐	☐
Anderes Land Welches?	☐ ☐	☐ ☐	☐ ☐

2. b) Falls ein Elternteil oder beide nicht in der Schweiz geboren wurden, seit wie vielen Jahren leben Sie und Ihre Eltern/Erziehungsberechtigten in der Schweiz? Falls die Eltern/Erziehungsberechtigten in der Schweiz geboren wurden, bitte leer lassen.

Ihr Vater seit ☐☐ Jahren

Ihre Mutter seit ☐☐ Jahren

Sie seit ☐☐ Jahren

3. Welche Sprache sprechen Sie in der Familie?

☐ Schweizerdeutsch
☐ Hochdeutsch
☐ Französisch
☐ Italienisch
☐ Rätoromanisch
☐ Spanisch
☐ Portugiesisch
☐ Südslawisch (Bosnisch, Kroatisch, Serbisch, Mazedonisch, Slowenisch)

☐ Albanisch
☐ Türkisch
☐ Englisch
☐ Skandinavisch (Norwegisch, Dänisch, Schwedisch)
☐ Andere Sprache, welche?

4. Welchen höchsten Bildungsabschluss haben Ihre Eltern/Erziehungsberechtigten?
Bitte in jeder Spalte ein Kästchen ankreuzen.

	Ihr Vater bzw. Ihre männliche Bezugsperson (z.B. Stief- oder Pflegevater)	Ihre Mutter bzw. Ihre weibliche Bezugsperson (z.B. Stief- oder Pflegemutter)
Doktorat	☐	☐
Universitätsabschluss, Fachhochschulabschluss, Abschluss an einer Pädagogischen Hochschule	☐	☐
Höhere Fach- und Berufsbildung (z.B. eidg. Fachausweis, Meisterdiplom)	☐	☐
Maturität	☐	☐
Fachmittelschule, Berufslehre oder Berufsschule	☐	☐
Abschluss der Sekundarstufe I	☐	☐
Primarschulabschluss	☐	☐
Keinen Primarschulabschluss	☐	☐

5. Welchen Beruf übt Ihr Vater bzw. Ihre männliche Bezugsperson (z.B. Stief- oder Pflegevater) aus?
(z.B. Lehrer, Küchenhilfe, Verkaufsleiter)

Geben Sie seinen letzten Beruf an, sofern er im Moment nicht arbeitet. Beschreiben Sie, was er derzeit tut, wenn er niemals einen Beruf gehabt hat.

6. Was macht Ihr Vater bzw. Ihre männliche Bezugsperson (z.B. Stief- oder Pflegevater) in seinem Beruf?
(z.B. er unterrichtet Schüler eines Gymnasiums oder einer Realschule, er hilft in einem Restaurant bei der Zubereitung von Mahlzeiten, er leitet ein Verkaufsteam)

Beschreiben Sie in einem Satz, was er in seinem Beruf macht, oder gemacht hat.

7. Welchen Beruf übt Ihre Mutter bzw. Ihre weibliche Bezugsperson (z.B. Stief- oder Pflegemutter) aus?
(z.B. Lehrerin, Küchenhilfe, Verkaufsleiterin)

Geben Sie ihren letzten Beruf an, sofern sie im Moment nicht arbeitet. Beschreiben Sie, was sie derzeit tut, wenn sie niemals einen Beruf gehabt hat.

8. Was macht Ihre Mutter bzw. Ihre weibliche Bezugsperson (z.B. Stief- oder Pflegemutter) in ihrem Beruf?
(z.B. sie unterrichtet Schüler eines Gymnasiums oder einer Realschule, sie hilft in einem Restaurant bei der Zubereitung von Mahlzeiten, sie leitet ein Verkaufsteam)

Beschreiben Sie in einem Satz, was sie in ihrem Beruf macht, oder gemacht hat.

9. In welcher beruflichen Stellung sind Ihre Eltern/Erziehungsberechtigten tätig?
Wenn sie zur Zeit nicht berufstätig sind, geben Sie bitte an, welche berufliche Stellung sie in ihrem letzten Beruf hatten.

Bitte in jeder Spalte nur ein Kästchen ankreuzen.	Ihr Vater bzw. Ihre männliche Bezugsperson (z.B. Stief- oder Pflegevater)	Ihre Mutter bzw. Ihre weibliche Bezugsperson (z.B. Stief- oder Pflegemutter)
Selbständige/r	☐	☐
Freiberuflich tätige/r Akademiker/in	☐	☐
Mithelfende/r Familienangehörige/r	☐	☐
Beamter/Beamtin	☐	☐
Angestellte/r	☐	☐
Arbeiter/in	☐	☐
Die Person ist nie berufstätig gewesen	☐	☐

10. Wie viele Bücher haben Sie ungefähr zu Hause?

Keine Bücher	☐	51-100 Bücher	☐
1-10 Bücher	☐	101-200 Bücher	☐
11-25 Bücher	☐	201-500 Bücher	☐
26-50 Bücher	☐	Mehr als 500 Bücher	☐

Appendix 3: Comparing and Contrasting Teaching Material

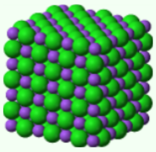
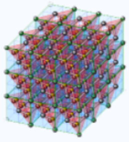
Note: The solutions to the worksheets are not presented in this dissertation. They can, however, be requested from the author.

The detailed assignment of the learning activities to different methods is depicted in Table 2.

Table 2: Classification of Learning Activities of the Comparing and Contrasting Teaching Material

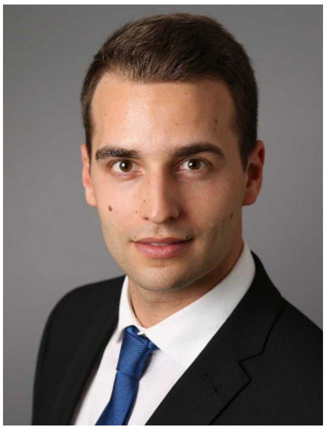
Chapter	Worksheet	Content	compare*	compare and contrast*	experiment using CC*	ICC	HMMC	Interleaved practice*	Making use of analogy*	pre-structured concept map	self-explanations	cognitively activiating introduction	productive failure	common practice	training of procedural knowledge
0		Introduction of the coulomb law - basis for the understanding of chemical bonds													
1	1	Comparison of ice, sodiumchloride crystal and diamond		1	1	1									
1	2	Introduction to Electronegativity with three different elements (Li, F, Cl)	1	1		1									
1	Reading	Analogy: Electron thieves and victims		1					1						
1	Overview Sheet	Three types of bonding overview graphic		1											
1	3	Three types of bonding - worksheet for practice		1				1							
1	4	Self-explanations of concepts learned									1				
2	1	Conductivitiy experiment part I (Tap water, pure water, NaCl (s), NaCl in water)	1	1	1										
2	2	From the atom to the ion												1	
2	3	Formation of an ionic lattice	1	1		1									
2	4	Holistic mental model confrontation: Structure of NaCl		1			1								
2	5	Molecular formula of sodium chloride										1			
2	6	Explanation of the presence of full shells for ions in ionic compounds												1	
2	Chapter 2.2	Names and formulas of ionic compounds													1
2	7	Comparisons of melting points of different salts	1	1		1									
2	8	Pre-structured concept maps for ionic compounds / ionic bonding								1					
3	Chapter 3.1	Conductivity experiment part II (water, NaCl, NaCl in water, Aluminium foil)		1	1										
3	1	Comparison of ionic and metallic bonds: Cohesion after application of force on structre		1											
3	2	Self-explanations and exercices for the comparison of metallic and ionic substances		1							1				
3	3	Properties of metallic substances									1				
4	Chapter 4.1	Conductivity experiment part III (NaCl, Aluminium foil, ice, pure water)		1	1										
4	Chapter 4.3	Physical state at room temperature amd melting point (NaCl, Aluminium foil, water and hydrogen)		1	1										
4	1	worksheet for conductivity experiment		1	1										
4	2	The hydrogen atom (size and electron density)				1			1						
4	3	The hydrogen molecule (H2)												1	
4	Chapter 4.5.2	Two approaching hydrogen atoms: train analogy	1	1		1			1						
4	4	Questions for the understanding of the covalent bond in an hydrogen molecule (worksheet after train analogy)									1				
4	5	Introduction of noble gas principle using productive failure										1	1		
4	6	Worksheet on how to draw Lewis structures													1
4	6	Comparison of HCl with KCl (task 2 of worksheet 6)		1							1				
4	Chapter 4.6	Defintion of the term "molecule" and excercise		1				1							
4	Chapter 4.7	What information can be derived from a chemical formula - comparison of a metall, salt and molecule		1											
4	Chapter 4.8	Introcuction of polyatomic ions										1			
4	7	Formula and names of ionic compounds containing polyatomic ions - worksheet									1				1
4	8	Spatial arrangment of electron clouds	1	1		1									
4	9	Practice of the principle of VSEPR													1
4	10	Overview over 3 bonding types: pre-strucutured concept map		1						1					
5	1	Assigning of boiling temperatures of viarous substances (metallic, ionic and molecular substances)		1		1		1				1			
	Chapter 5.1	Introductory experiment with water jet deflection vs. heptane			1										
5	2	explanation of intermolecular forces in water												1	
5	Chapter 5.3	relative strength of intermolecular forces and chemical bonds		1											
5	3	dipole-dipole forces: comparision of three molecular substances' boilingpoints (methane, dichloromethane and chloroform)	1	1		1									
5	Chapter 5.7	hydrogen bonds - exercises with some molecular substances												1	
5	4	Worksheet on Van der Waals forces and comparison of all intermolecular forces	1	1		1									
5	5	Comparing a salt crystal with an ice crystal	1	1											
5	Chapter 5.10	Comparison of ice, sodiumchloride crystal and diamond		1											
		Number of activities counted:	**9**	**27**	**7**	**10**	**1**	**3**	**3**	**2**	**6**	**4**	**1**	**5**	**4**

Unterlagen zur chemischen Bindungslehre

Bindungsart	ionische Bindung	metallische Bindung	kovalente Bindung		
Art der Elemente	Metalle und Nichtmetalle	Metalle unter sich	Nichtmetalle unter sich		
Anziehung zwischen	Anionen und Kationen	Atomrümpfen + Elektronengas	Atomrümpfen + Elektronen		
Art der Teilchen oder Verbände	**riesiger Ionenverband,** Anordnung gemäss **Ionengitter**	**riesiger Atomverband,** Anordnung gemäss **Metallgitter**	kleine Moleküle	riesige Moleküle	**riesiger Atomverband,** Anordnung gemäss einem Atomgitter
Stoffklasse	salzartige Stoffe	metallische Stoffe	flüchtige Stoffe	hochmolekulare Stoffe	diamantartige Stoffe
Abbildungen					

Entwicklung der Unterrichtsmaterialien in Kooperation mit dem MINT-Lernzentrum der ETH Zürich: Dr. Adrian Zwyssig, Dr. Juraj Lipscher

Entwicklung der Unterrichtseinheit



Dr. Adrian Zwyssig
Chemiker, Chemielehrperson

Institut für empirische Lehr- und Lernforschung (Prof. Dr. E. Stern)
Laboratorium für Anorganische Chemie (Prof. em. Dr. A. Togni)

Dissertationsprojekt zur «Diagnose und Förderung des Verständnisses der chemischen Bindungslehre»

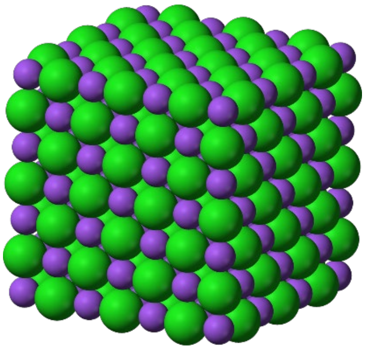
Dr. Juraj Lipscher
Chemiker, Chemielehrperson

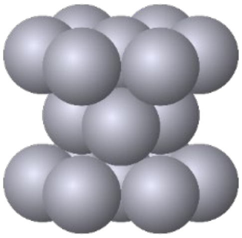
MINT-Lernzentrum, ETH Zürich

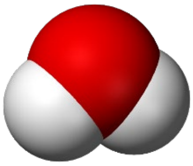
Bemerkungen

Die in dem Kurs verwendeten Unterrichtsmaterialien sind Teil des Dissertationsprojekts von Adrian Zwyssig. Die Unterrichtsmaterialien dürfen für den Eigengebrauch verwendet werden, jedoch dürfen diese weder verbreitet noch kommerziell verwendet werden.

I. Einführung in die drei Bindungsarten







Arbeitsblatt I/1: Struktur und Eigenschaften von Stoffen

In der untenstehenden Tabelle finden Sie die Abbildungen und die Schmelztemperaturen von drei ähnlich aussehenden Stoffen: Wasser (Eis), Kochsalz (Natriumchlorid NaCl) und Diamant (reiner Kohlenstoff).

Tab. 1: Eis, Natriumchlorid und Diamant (Rob Levinsky (n.b.)) mit den Schmelztemperaturen.

Wasser	**Natriumchlorid**	**Diamant**
H_2O	NaCl	C
		
Schmelztemperatur		
0 °C	801 °C	Etwa 4 000 °C

Frage: Wie ist es möglich, dass so ähnlich aussehende Stoffe so unterschiedliche Eigenschaften aufweisen? Überlegen Sie sich, welche Gemeinsamkeiten und Unterschiede auf der Ebene der Teilchen und Bindungen den Gemeinsamkeiten und Unterschieden bei den Stoffeigenschaften zugrunde liegen können.

- Welche strukturellen Merkmale könnten für das ähnliche Aussehen verantwortlich sein?
- Und mit welchen Beziehungen zwischen den Teilchen könnte man die Unterschiede bei den Schmelztemperaturen erklären?

Arbeitsblatt I/2: Elektronegativität

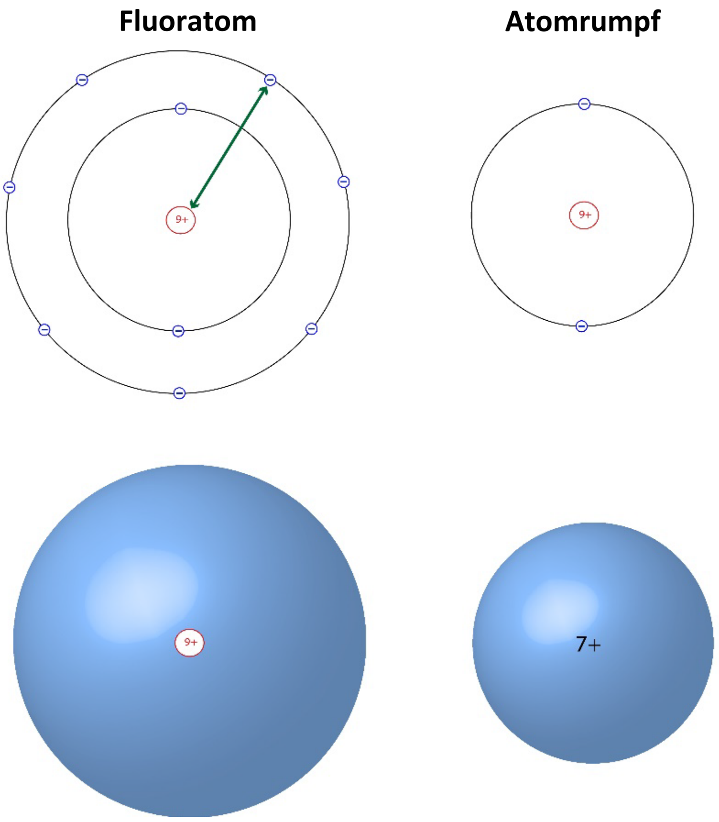
Sie haben bereits Einiges über den Aufbau der Atome verschiedener Elemente gelernt. Wir haben dabei aber oft nur einzelne Atome betrachtet. Im Folgenden wollen wir uns überlegen, was geschieht, wenn Atome verschiedener Elemente in einem Stoff enthalten sind. Hierbei ist es von grosser Bedeutung, wie stark ein Atom eigene Elektronen sowie die Elektronen anderer Atome anzieht. Wenn wir Atome verschiedener Elemente miteinander vergleichen, erhalten wir ein relatives Mass für diese Eigenschaft, die als Elektronegativität bezeichnet wird.

Definition

Die Elektronegativität ist ein relatives Mass dafür, wie stark Elektronen von einem Atom angezogen werden.

Abschirmung und Atomrumpfladung

Möchte man die Anziehung eines Valenzelektrons zu seinem Atomkern berechnen, so muss beachtet werden, dass zwischen dem Valenzelektron und dem Kern innere Elektronen liegen, welche die vom Elektron erfahrene positive Ladung des Atomkerns abschirmen und damit verringern. Die effektive Ladung, die beispielsweise ein Valenzelektron eines Fluoratoms erfährt, ist demnach nicht 9+, sondern nur 7+. Formal lässt sich ein Atom in den ***Atomrumpf*** und seine Valenzelektronen aufteilen. Entsprechend spricht man auch von einer ***Atomrumpfladung*** von 7+.



+ 7 Valenzelektronen

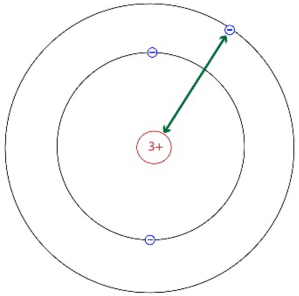
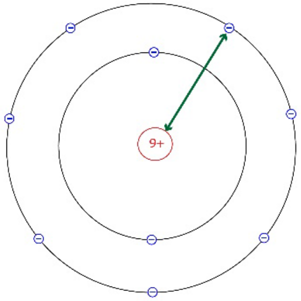
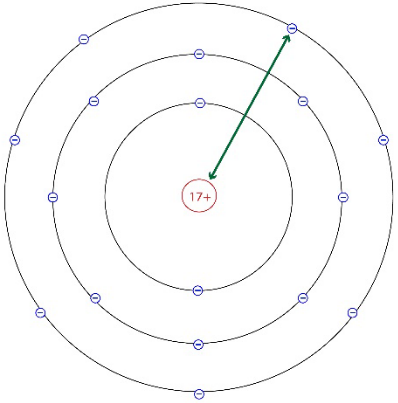
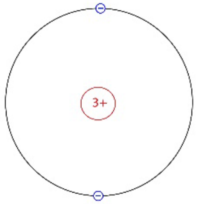
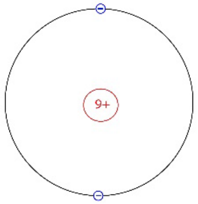
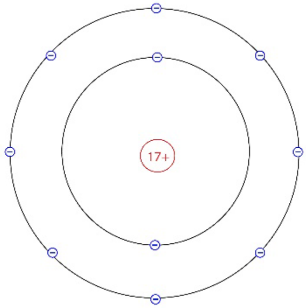
9 Protonen

2 innere Elektronen (Abschirmung)

resultierende Atomrumpfladung: 7+

Auftrag 1: Berechnen Sie die Atomrumpfladung eines Lithium- und Chloratoms und tragen Sie die Anzahl der Valenzelektronen in Tabelle 1 ein.

Tab 1: Atomrumpfladungen und Elektronegativitätswerte von Li, F und Cl.

	Lithiumatom	**Fluoratom**	**Chloratom**
neutrale Atome im Schalenmodell			
Atomrumpf			
Atomrumpfladung		7+	
Valenzelektronen			
Elektronegativitätswert	1.0	4.0	3.2

Auftrag 2: Formulieren Sie eine einfache Regel, welche es uns erlaubt, die Atomrumpfladung für ein beliebiges Element zu ermitteln.

Auftrag 3: Ein Lithiumatom hat einen tieferen Elektronegativitätswert (1.0) als ein Fluoratom (4.0). Erklären Sie mit dem Coulombgesetz, weshalb ein Fluoratom Elektronen stärker anzieht.

Auftrag 4: Chlor- und Fluoratome haben die gleiche Atomrumpfladung, dennoch weisen Chloratome eine tiefere Elektronegativität auf. Können Sie dies mit dem Coulombgesetz erklären?

Auftrag 5: Im Periodensystem nimmt die Elektronegativität von links nach rechts zu und von oben nach unten ab. Können Sie dies mit dem Coulombgesetz erklären?

Auftrag 6: Überlegen Sie sich, wo sich im Periodensystem metallische und nichtmetallische Elemente befinden und versuchen Sie, eine Faustregel bezüglich ihrer Elektronegativitätswerte aufzustellen.

Nichtmetalle haben in der Regel ______________ Elektronegativitätswerte.

Metalle haben in der Regel ______________ Elektronegativitätswerte.

Auftrag 7: Für die in einem Stoff herrschenden Anziehungskräfte spielt es eine Rolle, ob Atome mit tiefen Elektronegativitätswerten (typischerweise metallische Atome) und/oder solche mit hohen Elektronegativitätswerten (nichtmetallische Atome) enthalten sind. Welche Kombinationsmöglichkeiten zwischen den zwei Gruppen «Metalle» und «Nichtmetalle» gibt es?

Das Verständnis der drei Bindungsarten auf der Grundlage der Elektronegativität

Im Folgenden werden die drei Bindungsarten: ionische, metallische und kovalente Bindung, auf der Grundlage des Konzepts der Elektronegativität mithilfe der Analogie von Elektronenräubern und –opfern erläutert.

Um verstehen zu können, wie einzelne Atome überhaupt Bindungen mit anderen Atomen eingehen können, ist es zentral, wie stark ein Atom eigene Elektronen sowie die Elektronen anderer Atome anzuziehen vermag.

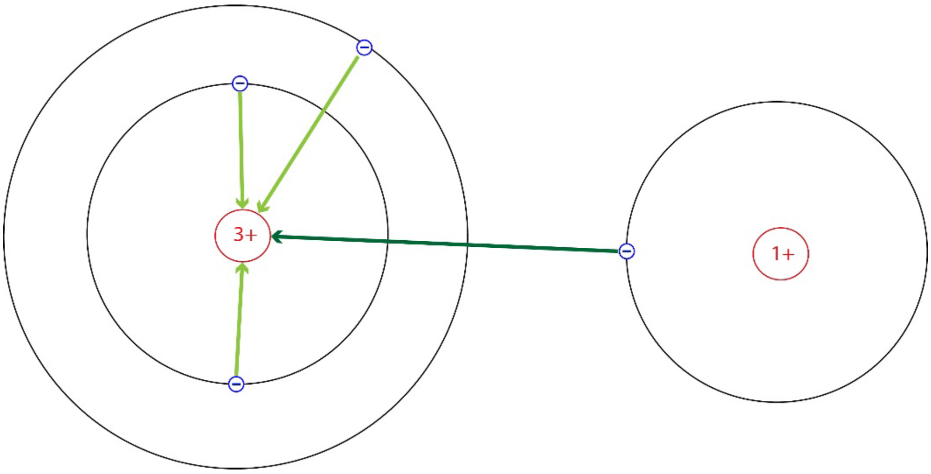


Abb. 1 Visualisierung der Anziehung eigener (hellgrün) und fremder Elektronen (dunkelgrün)

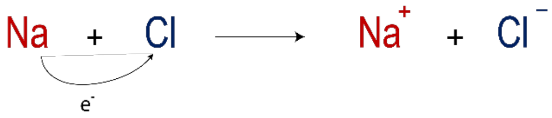
Wenn wir Atome verschiedener Elemente miteinander vergleichen, erhalten wir ein relatives Mass für diese Eigenschaft, die als Elektronegativität bezeichnet wird.

Definition: ***Die Elektronegativität ist ein relatives Mass dafür, wie stark Elektronen von einem Atom angezogen werden.***

Elemente mit hoher Elektronegativität werden als Elektronenräuber und Elemente mit niedriger Elektronegativität als Elektronenopfer bezeichnet.

1. Ionische Bindung: Elektronenopfer (Metalle) und Elektronenräuber (Nichtmetalle)

Die Situation, die sich beim Zusammentreffen eines Räubers mit einem Opfer ergibt, ist denkbar einfach: Das Opfer wird seiner Habseligkeiten beraubt und der Räuber wird reicher. Begegnungen von Elektronenräubern und Elektronenopfern führen demnach dazu, dass dem Metallatom seine Valenzelektronen vom Nichtmetallatom entrissen werden. Diese Elektronenübertragung führt zur Bildung eines positiv und eines negativ geladenen Ions.



$$\underbrace{Na + Cl}_{e^-} \longrightarrow Na^+ + Cl^-$$

Die auf diese Weise entstandenen Ionen ordnen sich so an, dass sich entgegengeladene Ionen möglichst nahekommen. Ein solcher Zusammenhalt der Ionen durch elektrostatische Anziehung zwischen entgegengesetzt geladenen Ionen wird als ionische Bindung bezeichnet.

Es ist ganz wichtig hervorzuheben, dass dieser Prozess typischerweise nicht nur mit zwei Atomen, das heisst einem Elektronenräuber und einem Elektronenopfer, sondern mit vielen Atomen gleichzeitig passiert. Dies führt dazu, dass wir nicht nur ein Ionenpaar, sondern einen grossen Verbund von Ionen erhalten.

Neben der Anziehung entgegengeladener Ionen gibt es auch noch die Abstossung gleichgeladener Ionen. Während die entgegengeladenen Ionen bestrebt sind, einander möglichst nahe zu kommen, sind die gleichgeladenen Ionen bestrebt, möglichst viel Abstand zueinander zu halten. Aus dem Zusammenwirken beider Faktoren ergibt sich eine gitterförmige Anordnung beider Ionensorten, die man als Ionengitter bezeichnet. Auf diese Weise entstehen riesige, unbestimmt grosse Ionenverbände.

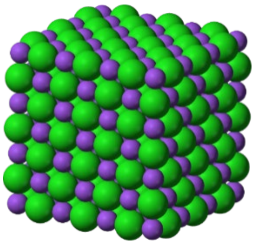


Abb. 2 Ionengitter

Da metallische Atome oft in der Rolle der Elektronenopfer sind, ist die Fehlvorstellung weit verbreitet, die Atome von Metallen würden von sich aus ihre Valenzelektronen abgeben. Diese Vorstellung ist falsch. Um Valenzelektronen entgegen der Anziehung zum Atomkern zu entfernen, muss auch bei metallischen Atomen Ionisierungsenergie aufgewendet werden. Die Ionisierungsenergie der Atome metallischer Elemente ist zwar geringer als bei den Atomen nichtmetallischer Elemente, aber sie ist trotzdem beträchtlich. Natrium weist beispielsweise eine erste Ionisierungsenergie von 5,14 eV (495,8 kJ/mol) auf. Dies wiederlegt die Idee der «freiwilligen Abgabe» von Valenzelektronen ganz eindeutig. Die korrekte Sichtweise ist demnach: Die Atome metallischer Elemente (Elektronenopfer) ziehen ihre Elektronen nicht allzu stark an, sodass ihnen diese von den Atomen der Nichtmetalle (Elektronenräuber) verhältnismässig leicht entrissen werden können.

Dieser Zusammenhang lässt sich wiederum mit der Analogie von Elektronenräubern und -opfern erläutern: Die Menschen, die ihr Hab und Gut nicht besonders stark verteidigen können oder wollen, die wir als Opfer bezeichnet haben, sind sicherlich nicht bestrebt, ihre Besitztümer dem Räuber freiwillig abzugeben. Es ist vielmehr so, dass sie zu schwach sind, um ihr Eigentum gegen die Räuber zu verteidigen.

2. Metallische Bindung: Elektronenopfer (Metalle) untereinander

Treffen zwei oder mehrere Elektronenopfer aufeinander, die ihre Valenzelektronen nicht besonders stark verteidigen können, so werden sie sich ihren Besitz gegenseitig auch nicht streitig machen. Da sie sozusagen kein starkes Interesse an Besitztümern hegen, werden sie eher eine Gemeinschaft bilden, in der sie ihre Habseligkeiten gemeinsam nutzen.

Metallatome bilden ebenfalls riesige, unbestimmt grosse Atomverbände, ähnlich wie wir es bei den ionischen Bindungen gesehen haben. Da sie aber ihre Elektronen nicht sehr stark anziehen, verlieren die Atome ihre Elektronen und werden dadurch zu positiv geladenen Atomrümpfen. Aus diesem Grund sind die Elektronen in einem metallischen Verband nicht zwischen zwei Atomen lokalisiert, wie es bei der kovalenten Bindung der Fall ist. Sie sind vielmehr im ganzen Atomverband verteilt und allen Atomen gemeinsam. Solche frei beweglichen Elektronen werden als Elektronengas bezeichnet. Die metallische Bindung besteht also in der Anziehung zwischen den positiv geladenen Atomrümpfen und dem Elektronengas.

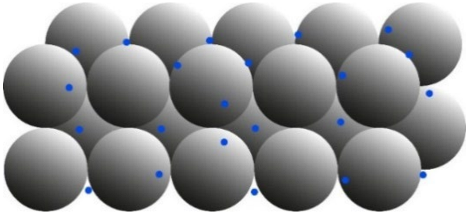


Abb. 3 einfaches Modell der metallischen Bindung

Da die Anziehung zwischen Atomrümpfen und Elektronengas eine Wechselwirkung ist, lässt sie sich natürlich auch so beschreiben, dass die Elektronen die Atomrümpfe anziehen. So gesehen lässt sich also auch sagen, dass das negativ geladene Elektronengas die positiv geladenen Atomrümpfe zusammenhält.

3. Kovalente Bindung: Elektronenräuber (Nichtmetalle) untereinander

Treffen zwei oder mehrere gleich starke Räuber aufeinander, so können sie sich gegenseitig ihre Beute nicht streitig machen, sie müssen diese vielmehr untereinander aufteilen. Verbinden sich beispielsweise zwei Chloratome miteinander, so ziehen beide Atomkerne die Valenzelektronen beider Atome an. Diese Anziehung der Valenzelektronen durch beide Kerne führt dazu, dass die Atome in einem kleinen Abstand zueinander bleiben. Diese Art chemischer Bindung wird als kovalente Bindung bezeichnet [lat. *co(n)* = mit, *valentia* = Kraft, Stärke].

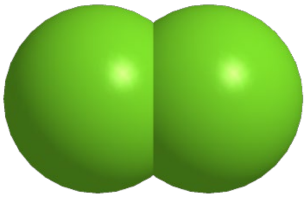


Abb. 4 Zwei Chloratome bilden ein Chlormolekül

Kovalente Bindungen zwischen Atomen können zur Ausbildung von Atomgruppen führen, die man als Moleküle bezeichnet [lat. *moles* = Masse, *molecula* = diminutiv von moles]. Wasser (H_2O) beispielsweise besteht aus Wassermolekülen, die ein Sauerstoffatom und zwei Wasserstoffatome enthalten. Die einzelnen Atome in einem solchen Molekül werden durch kovalente Bindungen zusammengehalten.

Tabelle 1: Die drei Bindungsarten (Schülerversion am Anfang)

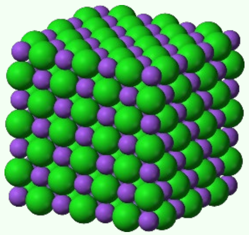
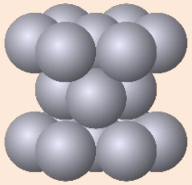
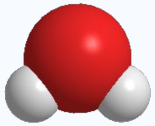
Bindungsart	**ionische Bindung**	**metallische Bindung**	**kovalente Bindung**		
Art der Elemente	**Metalle und Nichtmetalle**	**Metalle unter sich**	**Nichtmetalle unter sich**		
Anziehung zwischen	**Anionen und Kationen**	**Atomrümpfen + Elektronengas**	**Atomrümpfen + Elektronen**		
Art der Teilchen oder Verbände	**riesiger Ionenverband,** Anordnung gemäss **Ionengitter**	**riesiger Atomverband,** Anordnung gemäss **Metallgitter**	**kleine Moleküle**		
Stoffklasse					
Abbildungen					

Tabelle 4: Die drei Bindungsarten (Endversion)

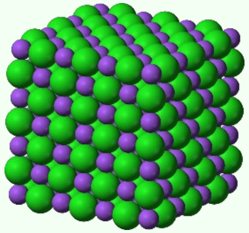
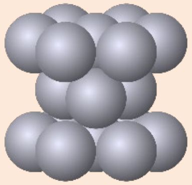
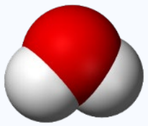
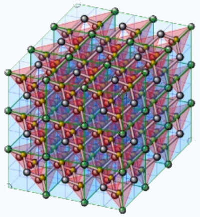
Bindungsart	**ionische Bindung**	**metallische Bindung**	**kovalente Bindung**		
Art der Elemente	**Metalle und Nichtmetalle**	**Metalle unter sich**	**Nichtmetalle unter sich**		
Anziehung zwischen	**Anionen und Kationen**	**Atomrümpfen + Elektronengas**	**Atomrümpfen + Elektronen**		
Art der Teilchen oder Verbände	**riesiger Ionenverband,** Anordnung gemäss **Ionengitter**	**riesiger Atomverband,** Anordnung gemäss **Metallgitter**	**kleine Moleküle**	**riesige Moleküle**	**riesiger Atomverband,** Anordnung gemäss einem Atomgitter
Stoffklasse	**salzartige Stoffe**	**metallische Stoffe**	**flüchtige Stoffe**	**hochmolekulare Stoffe**	**diamantartige Stoffe**
Abbildungen					

Tabelle 5: Bindungsarten bei verschiedenen Arten von Elementen

<table>
<tr><td></td><td colspan="2">Metalle
(Opfer)</td><td colspan="2">Nichtmetalle
(Elektronenräuber)</td></tr>
<tr><td rowspan="2">Metalle
(Opfer)</td><td colspan="2">metallische Bindung</td><td colspan="2">ionische Bindung</td></tr>
<tr><td>Atomrümpfe + Elektronengas</td><td>riesiger Atomverband, Anordnung gemäss Metallgitter</td><td>Anionen + Kationen</td><td>riesiger Ionenverband, Anordnung gemäss Ionengitter</td></tr>
<tr><td rowspan="4">Nichtmetalle
(Elektronenräuber)</td><td colspan="2" rowspan="4"></td><td colspan="2">kovalente Bindung</td></tr>
<tr><td rowspan="3">neutrale Atome</td><td>kleine Moleküle</td></tr>
<tr><td></td></tr>
<tr><td></td></tr>
</table>

Arbeitsblatt I/3: Elektronenräuber und –opfer. Zuordnung der Bindungstypen

In der untenstehenden Tabelle finden Sie die Werte der Elektronegativitäten (EN) der wichtigsten Elemente. EN-Werte höher als 2 charakterisieren einen Elektronenräuber. Werte unterhalb von 2 deuten darauf hin, dass das Element zu den Elektronenopfern gehört.

H **2,1**						
Li **1,0**	**Be** **1,5**	**B** **2,0**	**C** **2,5**	**N** **3,0**	**O** **3,5**	**F** **4,0**
Na **0,9**	**Mg** **1,2**	**Al** **1,5**	**Si** **1,8**	**P** **2,1**	**S** **2,5**	**Cl** **3,0**
K **0,8**	**Ca** **1,0**	**Ga** **1,6**	**Ge** **1,8**	**As** **2,0**	**Se** **2,4**	**Br** **2,8**
Rb **0,8**	**Sr** **1,0**	**In** **1,7**	**Sn** **1,8**	**Sb** **1,9**	**Te** **2,1**	**I** **2,5**

Auftrag 1: Entscheiden Sie aufgrund der EN-Werte der beiden Bindungspartner, zu welcher Art die folgenden chemischen Bindungen gehören.

Bindungspartner	**Bindungsart**
Na und Br	[ ] Kovalente Bindung [ ] Ionenbindung [ ] Metallische Bindung
O und O	[ ] Kovalente Bindung [ ] Ionenbindung [ ] Metallische Bindung
Al und Al	[ ] Kovalente Bindung [ ] Ionenbindung [ ] Metallische Bindung
C und F	[ ] Kovalente Bindung [ ] Ionenbindung [ ] Metallische Bindung

Auftrag 2: Führen Sie zwei Bindungspartner auf, welche eine chemische Bindung mit den folgenden Merkmalen eingehen könnten. Die bereits aufgeführten Beispiele im Auftrag 1 sollten Sie nicht mehr aufführen.

Merkmale der chemischen Bindung	**Bindungspartner**
kovalente Bindung	
Metallische Bindung	
Ionenbindung	

Arbeitsblatt I/4: Selbsterklärungen von Grundkonzepten und Zusammenhängen

- Eine Mitschülerin argumentiert, dass gemäss dem Coulombgesetz die Anziehungskraft zwischen einem negativ geladenen Elektron und einem positiv geladenen Atomkern umso grösser wird, je höher die Anzahl der Protonen im Kern ist. Sie versteht deshalb nicht, wie der tiefe Elektronegativitätswert von 0.7 für ein Franciumatom mit 87 Protonen zustande kommt. Erkläre ihr, welche Faktoren sie bei ihren Überlegungen nicht berücksichtigt hat.
- Erklären Sie, wofür man das Konzept der Elektronegativität braucht.
- Erklären Sie die Unterscheidung zwischen den drei Bindungstypen anhand der Analogie von Elektronenräubern und –opfern.
- Hugo macht den Vorschlag, dass man für die Unterscheidung der Bindungsarten anstelle von Elektronenräubern und –opfern viel eher die Analogie von einem Gast und Gastgeber verwenden sollte. Welcher Aspekt wird beim Verwenden dieser Analogie falsch dargestellt?
- Ein Mitschüler glaubt, die Atome von Metallen wären bestrebt, ihre Valenzelektronen abzugeben. Mit welchen Argumenten können Sie ihn davon überzeugen, dass seine Ansicht falsch ist?

II. Ionische Bindung

Arbeitsblatt II/1: Wie können wir Unterschiede in der Leitfähigkeit von Stoffen erklären?

Ergebnisse der Versuche zur Leitfähigkeit verschiedener Stoffe:

Skizze				
Stoff	*Leitungswasser*	*reines Wasser*	*Natriumchlorid* *(Kochsalzkristall)*	*Natriumchlorid in Wasser*
elektrische Leitfähigkeit				
frei bewegliche Teilchen				

In diesem Arbeitsblatt geht es darum, Unterschiede in der Leitfähigkeit von Stoffen wie zum Beispiel reinem Wasser, Natriumchlorid (Kochsalz) und einer Kochsalzlösung zu erklären.

Elektrischer Strom: Wenn ein Stoff elektrischen Strom leiten soll, muss er frei bewegliche elektrisch geladene Teilchen enthalten. Diese Teilchen bewegen sich beispielsweise von einem Pol der Batterie zum anderen Pol. Ein solcher Strom der Teilchen wird als elektrischer Strom bezeichnet.

Wir haben bereits besprochen, dass für die elektrische Leitfähigkeit zwei Voraussetzungen erfüllt sein müssen:

1. Der Stoff muss elektrische geladene Teilchen enthalten.
2. Die elektrisch geladenen Teilchen müssen frei beweglich sein.

Auftrag 1: Reines Wasser ist bei Zimmertemperatur flüssig und es ist nicht elektrisch leitfähig. Welche Folgerungen ergeben sich daraus? Notieren Sie Ihre Folgerungen in der untenstehenden Tabelle.

Sind die kleinsten Teilchen in diesem Stoff frei beweglich? (ja/nein)	Sind die kleinsten Teilchen in diesem Stoff elektrisch geladen? (ja/nein)

Auftrag 2: Die Lösung von Natriumchlorid in Wasser ist bei Zimmertemperatur flüssig und elektrisch leitfähig. Welche Folgerungen ergeben sich daraus? Notieren Sie Ihre Folgerungen in der untenstehenden Tabelle.

Sind die kleinsten Teilchen in dieser Lösung frei beweglich? (ja/nein)	Enthält diese Lösung elektrisch geladene Teilchen? (ja/nein)

Auftrag 3: Festes Natriumchlorid ist bei Zimmertemperatur fest und nicht elektrisch leitfähig. Welche Folgerungen ergeben sich daraus? Berücksichtigen Sie bei dieser Aufgabe die Folgerungen aus dem Auftrag 2. Notieren Sie Ihre Folgerungen in der untenstehenden Tabelle.

Sind die kleinsten Teilchen in diesem Stoff frei beweglich? (ja/nein)	Enthält dieser Stoff elektrisch geladene Teilchen? (ja/nein)

Auftrag 4: Welche Aussagen können Sie auf der Grundlage Ihrer Überlegungen über den Aufbau von Natriumchlorid machen? Fassen Sie Ihre Überlegungen aus den vorhergehenden Aufträgen hier zusammen.

2.1 Entstehung der Ionen

Arbeitsblatt II/2: Vom Atom zum Ion

Auftrag 1: Kochsalz (Natriumchlorid) lässt sich auf unterschiedliche Arten erzeugen.

a) Geben Sie einen Prozess an, bei dem der Schritt der Erzeugung der Ionen und ihrer Zusammenlagerung unmittelbar aufeinanderfolgend stattfinden.

b) Geben Sie einen Prozess an, bei dem der Schritt der Erzeugung der Ionen und ihrer Zusammenlagerung zeitlich stark versetzt stattfinden.

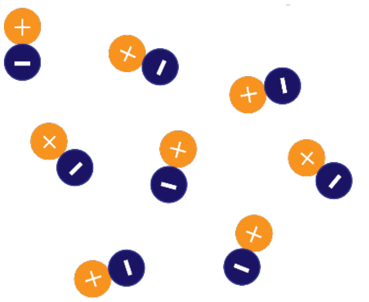
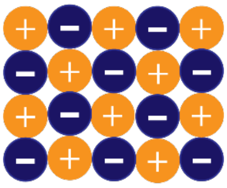
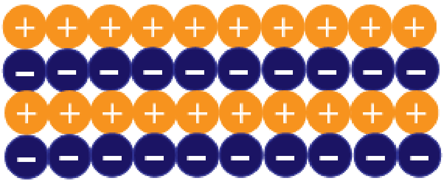
Auftrag 2: Ein Mitschüler gibt fälschlicherweise an, dass Natriumatome seine Valenzelektronen von sich aus abgeben, damit diese volle Schalen aufweisen. Argumentieren Sie mit den untenstehenden Werten, wie der Sachverhalt der Erzeugung von Natriumionen (Na^+) besser beschrieben werden kann. Sie dürfen auch mittels der Analogie von Elektronenräubern und Elektronenopfern argumentieren.

Element	**Elektronegativitätswert**	**1. Ionisierungsenergie kJ/mol**
Natrium (Na)	0.9	496
Chlor (Cl)	3.2	1256

Auftrag 3: Beschreiben Sie zwei Methoden, mit denen man Kochsalz (Natriumchlorid) im grossen Massstab gewinnen kann.

Arbeitsblatt II/3: Die Entstehung eines Ionengitters

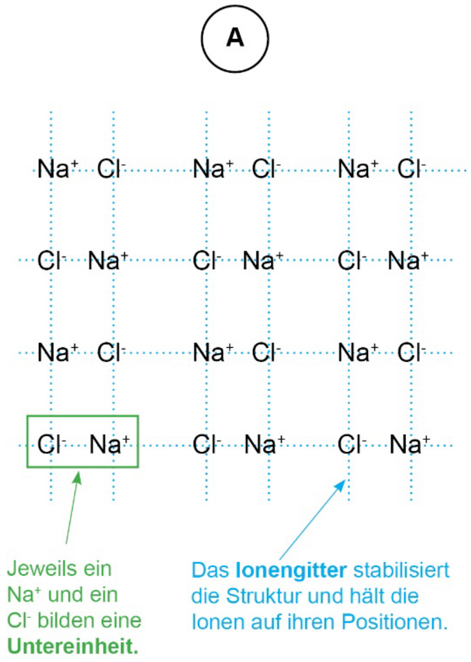
Auftrag 1: Im Folgenden geht es darum, sich zu überlegen, wie sich positiv und negativ geladene Ionen anordnen werden, wenn man sie zusammenbringt. Welche der folgenden Grafiken stellt aus Ihrer Sicht die zu erwartende Anordnung am besten dar? Kreuzen Sie die betreffende Grafik an und begründen Sie, weshalb Sie Ihre Wahl getroffen haben und wieso Sie die anderen Optionen ausgeschlossen haben.

A		**B**	
C		**D**	

	Begründung dafür oder dagegen
A	
B	
C	
D	

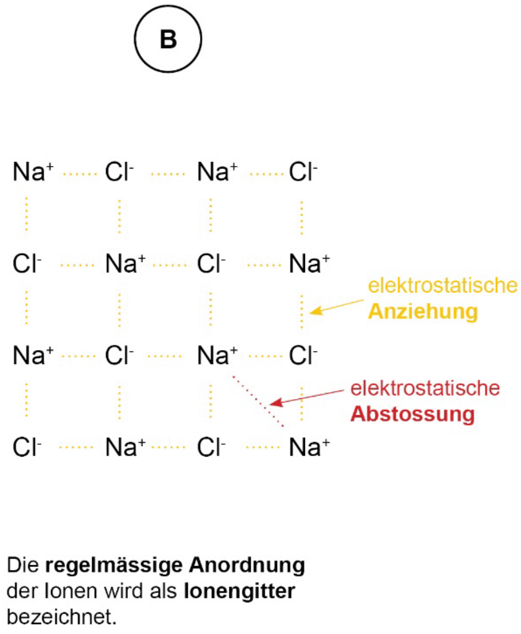
Arbeitsblatt II/4: Vergleich zweier Modelle eines Salzkristalls

Auftrag 1: Untenstehend sind zwei Modelle eines Kochsalzkristalls (Natriumchlorid, NaCl) dargestellt. Vergleichen Sie das im Unterricht kennengelernte Expertenmodell B mit dem fehlerhaften Modell A und beantworten Sie die folgenden Fragen.



Jeweils ein Na^+ und ein Cl^- bilden eine **Untereinheit.**

Das **Ionengitter** stabilisiert die Struktur und hält die Ionen auf ihren Positionen.



elektrostatische **Anziehung**

elektrostatische **Abstossung**

Die **regelmässige Anordnung** der Ionen wird als **Ionengitter** bezeichnet.

a) Welche Gemeinsamkeiten gibt es zwischen dem Modell A und dem Expertenmodell B?

b) Worin unterscheidet sich das Expertenmodell B von Modell A?

c) Welche Aspekte sind im Modell A falsch dargestellt?

Auftrag 2: Hugo empört sich über die Erläuterung der Lehrperson, dass das Ionengitter in Salzen nicht als ein physisch existierendes Gitter vorkommt, das die Ionen auf ihren Positionen hält.

a) Erkläre Hugo, was der Grund dafür ist, dass die Ionen zusammenhalten und bei Raumtemperatur kaum beweglich sind.

b) Erkläre Hugo, wieso man den Begriff des «Gitters» verwendet, indem du ihm erklärst, was das Ionengitter genau beschreibt.

Arbeitsblatt II/5: Summenformel von Natriumchlorid

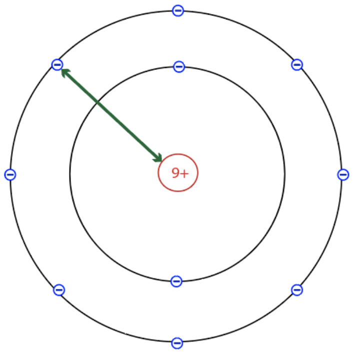
Auftrag 1: Kochsalz (Natriumchlorid) hat die Summenformel NaCl. Dennoch ist es falsch anzunehmen, dass jeweils ein Natrium-Kation und ein Chlor-Anion zusammen eine Untereinheit oder ein Paar bilden. Welchen Informationsinhalt lässt sich direkt aus der Summenformel ablesen?

Auftrag 2: Wie können Sie aus der Summenformel eines Stoffes herleiten, ob dieser Ionen enthält oder nicht?

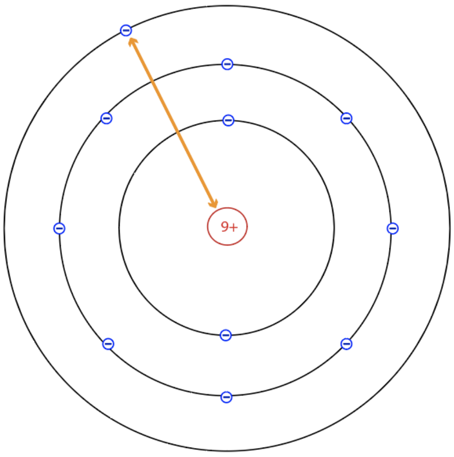
Arbeitsblatt II/6: Begründung für das Vorliegen von vollen Schalen bei Ionen in ionischen Verbindungen

Auftrag 1: Metallatome liegen in ionischen Verbindungen als Ionen vor, die sämtliche Valenzelektronen abgegeben haben. Können Sie mit dem Coulombgesetze erklären, warum Metallatomen nicht auch noch die Elektronen aus inneren Schalen entrissen werden?

Aufgabe 2: Anionen verfügen in ionischen Verbindungen über volle äussere Schalen. Bei Fluor bedeutet das, dass Fluor ein weiteres Elektron aufnimmt und ein F^--Anion bildet. Fluor besitzt aber von allen Elementen die höchste Elektronegativität und gehört damit zu den stärksten Elektronenräubern. Was spricht dagegen, dass ein F^--Anion ein weiteres Elektron aufnimmt und als F^{2-}-Anion vorliegt? Betrachten Sie dazu die beiden Anionen im Schalenmodell und argumentieren Sie mit Hilfe des Coulombgesetzes, warum aus einem F^{2-} leicht wieder ein F^--Anion werden kann.



F^-



F^{2-}

2.2 Formeln und Namen von Salzen

a) Formeln (Hauptgruppenelemente)

Bei **Hauptgruppenelementen** können die Ladungen der Ionen und somit auch die Formeln der Salze einfach ermittelt werden.

- Metallatome werden all ihrer Valenzelektronen beraubt.

- Nichtmetallatome haben ihre äusserte Schale auf acht aufgefüllt.

Kennt man die Ionenladungen, so kann man die beiden Ionen so kombinieren, dass das resultierende Salz elektrisch neutral wird.

Auftrag 1: vervollständigen Sie die Tabelle.

Metall	Anzahl Valenz-elektronen	Formel des Kations	Nicht-metall	Anzahl Valenz-elektronen	Formel des Anions	Formel des Salzes
Na	1	Na^+	**Cl**	7	Cl^-	**NaCl**
Mg			**Br**			
Ca			**O**			
Al			**S**			

b) Namen (Hauptgruppenelemente)

Salze, welche nur aus einatomigen Ionen bestehen, erhalten ihre Namen nach dem einfachen Schema:

Metall+Nichtmetall+id

NaCl → Natriumchlorid
$MgBr_2$ → Magnesiumbromid

Bei einigen Elementen der Nichtmetalle verwendet man die internationalen Namen der Elemente.

C^{4-} : Carbid	N^{3-} : Nitrid	O^{2-} : Oxid	F^- : Fluorid
	P^{3-} : Phosphid	S^{2-} : Sulfid	Cl^- : Chlorid
		Se^{2-} : Selenid	Br^- : Bromid
			I^- : Iodid

Auftrag 2: Füllen Sie die untenstehende Tabelle aus.

Verhältnisformel des Salzes	Name des Salzes	Formel des Kations	Formel des Anions
NaCl	Natriumchlorid	Na^+	Cl^-
K_2O			
BeO			
	Magnesiumbromid		
	Aluminiumoxid		
		Mg^{2+}	N^{3-}
	Berylliumcarbid		
		Na^+	Se^{2-}
	Magnesiumphosphid		

c) Nebengruppenelemente

Formel

Bei Nebengruppenelementen ist die Situation ein wenig komplizierter. Die Atome dieser Elemente weisen eine in der Regel unvollständig gefüllte d-Unterschale in der zweitäussersten Schale auf. Somit können sie auch Elektronen aus der zweitäussersten Schale abgeben, was dann zur Folge hat, dass sie mehrere verschieden geladene Ionen bilden können.

Kupfer bildet beispielsweise zwei verschiedene Ionen aus: Cu^+ und Cu^{2+} (Cu_2O und CuO)

Benennung

Bei Nebengruppenelementen müssen wir naturgemäss angeben, welche Ionen im Salzgitter vorliegen. Die Ladung des Kations wird hierbei mit einer sich in **Klammern befindlichen römischen Ziffer bezeichnet**. Bei der Ziffer in der Klammerhandelt es sich um die Ionenladung des Kations und nicht um den Index in der Formel.

Auftrag 3: Vervollständigen Sie die folgende Tabelle.

Verhältnisformel des Salzes	Name des Salzes	Formel des Kations	Formel des Anions
Cu_2O	Kupfer(I)-oxid	Cu^+	O^{2-}
CuO	Kupfer(II)-oxid	Cu^{2+}	O^{2-}
		Fe^{2+}	Cl^-
	Eisen(III)-chlorid		
Cu_3P			
		Ni^{2+}	O^{2-}

2.3 Erklärung der Freisetzung von Energie bei der Entstehung von ionischen Verbindungen

Experiment: Magnesiumband anzünden

Frage: Was ist der Grund für das starke Leuchten und die entstehende Wärme? Woher kommt diese Energie?

Arbeitsblatt II/7: Schmelzpunkte verschiedener Salze

Auftrag 1: In der untenstehenden Tabelle sind die Schmelzpunkte in °C bei Atmosphärendruck angegeben. Können Sie eine Tendenz erkennen, wenn wir ausschliesslich Salze mit einfach geladenen Ionen betrachten? Was könnte der Grund sein für die Unterschiede in den Schmelzpunkten?

	Cl^-	**Br^-**	**I^-**
Na^+	801	747	660
K^+	770	734	

Auftrag 2: Betrachten Sie wiederum die Schmelzpunkte der verschiedenen Salze. Können Sie eine Tendenz erkennen, wenn wir Salze mit einfach sowie mehrfach geladenen Ionen betrachten?

	F^-	**O^{2-}**
Na^+	993	1275
Mg^{2+}	1423	2852

Auftrag 3: Versuchen Sie abschliessend zu erklären, weshalb Natriumchlorid (NaCl) einen deutlich tieferen Schmelz- und Siedepunkt aufweist als Magnesiumoxid (MgO).

	Schmelzpunkt [°C] (1 bar)	**Siedepunkt [°C]** (1 bar)
NaCl	801	1465
MgO	2852	~ 3600

2.4 Zusammenfassung

Identifizierung ionischer Verbindungen

Ionische Verbindungen bilden sich bei Vorliegen von metallischen sowie nichtmetallischen Elementen in einer Substanz.

Ionenbildung

The Stärke der Anziehung von Elektronen ist durch die Elektronegativität charakterisiert. Wenn wir metallische wie auch nichtmetallische Elemente in einem Stoff präsent haben bringen wir zwei Extreme zusammen: Nichtmetalle mit hohen Anziehungskräften für die eigenen aber auch fremden Elektronen und Metalle mit eher geringen Anziehungskräften ihrer Valenzelektronen. Dabei wird dem metallischen Atom ein Elektron entrissen und dem nichtmetallischen Atom hinzugefügt. Dabei werden die zuvor neutralen Atome elektrisch geladen. Diese geladenen Teilchen werden als Ionen bezeichnet.

Definition eines Ions: Ein Ion ist ein elektrisch geladenes Teilchen.
Ein Ka**t**ion ist ein positives geladenes Teilchen. Ein Anion ist negativ geladen.

Ionen können durch das Entreissen oder Hinzufügen von Elektronen entstehen:
z.B. $Na \rightarrow Na^+$ oder $Cl \rightarrow Cl^-$

Entstehung ionischer Verbindungen

1. Schritt: **Elektronentransfer** vom metallischen Atom zum nichtmetallischen (Ionenbildung)

2. Schritt: **Anordnung der gebildeten Ionen** mit optimierten Anziehungs- und minimierten Abstossungskräften.

Bemerkung: Der erste und der zweite Schritt können, müssen aber nicht kurz nacheinander geschehen. Diese Prozesse können auch zeitlich weit auseinanderliegend stattfinden. Ein Beispiel hierfür ist die Bildung von Natriumchlorid-Kristallen beim Verdunsten von Meerwasser. Die Ionen waren bereits sehr lange im Meerwasser vorhanden, bevor der Prozess der Verdunstung und anschliessender Zusammenlagerung der Ionen stattgefunden hat.

Chemische Formel ionischer Verbindungen

Die chemische Formel ionischer Verbindungen enthalten Informationen zum Verhältnis der im Stoff vorhandenen Elemente. Es ist wichtig, dass man beachtet, dass die in der Formel vorhanden Elemente nicht als neutrale Atome vorliegen, sondern positiv und negativ geladen sind. Dies ist nicht selbstverständlich, weil dies in der chemischen Formel nicht so dargestellt wird (z.B. Na^+ statt Na-Atome in NaCl). Zusätzlich soll beachtet werden, dass auch wenn die Formel NaCl als Zweierpaar darstellt, es keine solche Untereinheiten gibt in einem Natriumchlorid-Kristall.

Nomenklatur ionischer Verbindungen

Siehe Kapitel 2.2

Regelmässige Anordnung und Ionengitter

The Optimierung der Anziehungs- und Minimierung der Abstossungskräften führt zur symmetrischen und regelmässigen Anordnung der Ionen.

Diese regelmässige Anordnung der Ionen in einer ionischen Verbindung wird als **Ionengitter** bezeichnet. Der Grund für die Anziehung der Ionen kommt aufgrund der Anziehung positiver und negativer Ladungen der Anionen und Kationen und nicht wegen dem Ionengitter zustande.

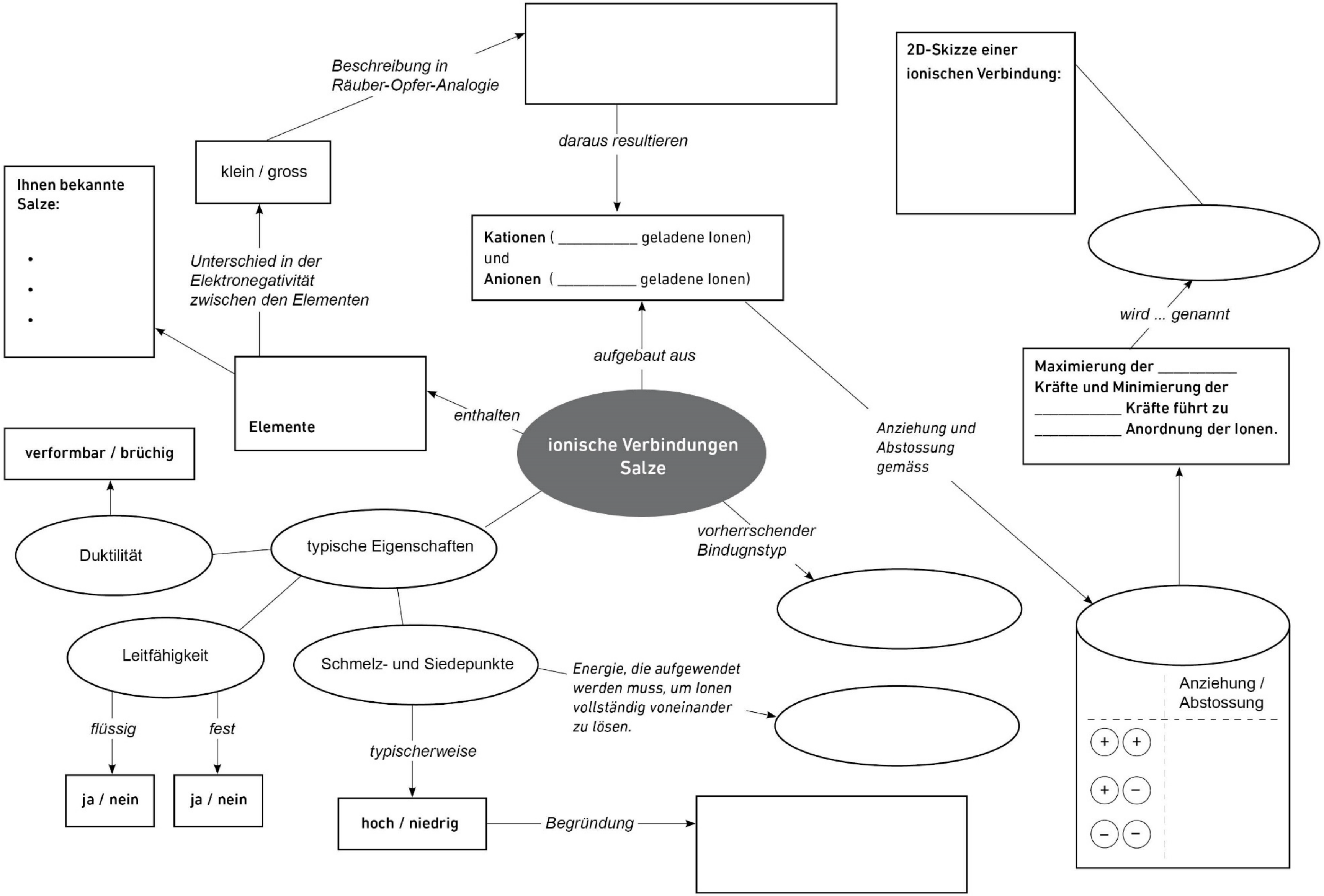
Die Stärke der Anziehung der Ionen ist von zwei Faktoren abhängig:

1. Höhe der Ladung (je grösser desto stärker)

2. Grösse der Ionen (je kleiner desto stärker)

Schmelz- und Siedetemperaturen ionischer Verbindungen

Die benötigte Energie, um die einzelnen Ionen voneinander zu lösen, ist von der Stärke der Anziehung der Ionen in einem Salz abhängig. Deshalb sind die Schmelz- respektive die Siedetemperaturen auch davon abhängig, wie stark diese Kräfte in einer ionischen Verbindung sind. Je stärker die Anziehungskräfte, desto mehr Energie muss aufgewendet werden, um den vorliegenden Anziehungskräften entgegenzuwirken, desto höher liegen auch die Schmelz- und Siedetemperaturen.


Beschreibung in Räuber-Opfer-Analogie
2D-Skizze einer ionischen Verbindung:
klein / gross
daraus resultieren
Ihnen bekannte Salze:
•
•
•
Unterschied in der Elektronegativität zwischen den Elementen
Kationen (__________ geladene Ionen) und Anionen (__________ geladene Ionen)
wird ... genannt
aufgebaut aus
Maximierung der __________ Kräfte und Minimierung der __________ Kräfte führt zu __________ Anordnung der Ionen.
Elemente
enthalten
Anziehung und Abstossung gemäss
verformbar / brüchig
ionische Verbindungen Salze
vorherrschender Bindugnstyp
Duktilität
typische Eigenschaften
Leitfähigkeit
Schmelz- und Siedepunkte
Energie, die aufgewendet werden muss, um Ionen vollständig voneinander zu lösen.
Anziehung / Abstossung
+ +
+ −
− −
flüssig
fest
ja / nein
ja / nein
typischerweise
hoch / niedrig
Begründung

III. Metallische Bindung

3.1 Ergebnisse der Versuche zur Leitfähigkeit verschiedener Stoffe:

Skizze				
Stoff	*reines Wasser*	*Natriumchlorid (Kochsalzkristall)*	*Natriumchlorid in Wasser*	***Aluminiumblech***
elektrische Leitfähigkeit				
frei bewegliche Teilchen (Ja/nein)				
Schmelzpunkt			-	

3.1.1 Folgerungen

3.1.2 Offene Fragestellungen

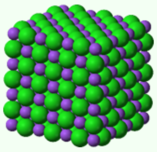
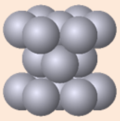
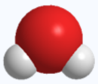
F1: Welche geladenen Teilchen sind frei beweglich bei festen metallischen Stoffen?

F2: Wie liegen die Atome in festen Metallen vor?

F3: Wie halten die Metallatome zusammen?

Sie sind hier

3.2 Übersicht

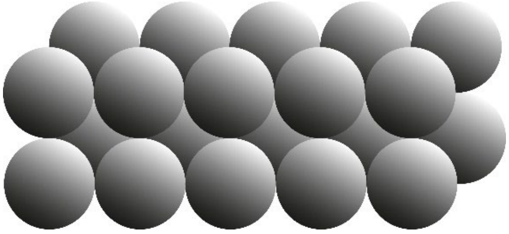
Bindungsart	ionische Bindung	metallische Bindung	kovalente Bindung		
Art der Elemente	Metalle und Nichtmetalle	Metalle unter sich	Nichtmetalle unter sich		
Anziehung zwischen	Anionen und Kationen	Atomrümpfen + Elektronengas	Atomrümpfen + Elektronen		
Art der Teilchen oder Verbände	**riesiger Ionenverband,** Anordnung gemäss **Ionengitter**	**riesiger Atomverband,** Anordnung gemäss **Metallgitter**	kleine Moleküle		
Stoffklasse					
Abbildungen					

3.3 Das Elektronengasmodell

Wir werden zuerst die Leitfähigkeit einiger Stoffe die Lupe nehmen. Zu den bereits im letzten Kapitel untersuchten Stoffen nehmen wir jetzt noch einen metallischen Stoff hinzu.

Ein Stoff muss frei bewegliche elektrisch geladene Teilchen enthalten, damit er elektrischen Strom leiten kann. Die Leitfähigkeit von Aluminium im festen Zustand legt den Schluss nahe, dass Metalle bereits im festen Zustand frei bewegliche elektrisch geladene Teilchen enthalten müssen. Diese Erkenntnis werden wir in der Folge nutzen, um das Wesen der metallischen Bindung zu ergründen.

Wir wollen uns als Erstes vorstellen, wie beispielsweise die Aluminiumatome in einem Stück Aluminiummetall angeordnet sind.

	
Metallisches Aluminium	Die regelmässige Anordnung der Aluminiumatome wird als *Metallgitter* bezeichnet.

Da die Atome elektrisch neutral sind im festen Zustand auch nicht frei beweglich sind, können wir die elektrische Leitfähigkeit von Aluminium mit dem oben gezeigten einfachen Modell nicht erklären.

Im nächsten Schritt werden wir die Elektronegativität von Aluminium mit derjenigen von Sauerstoff und Fluor vergleichen.

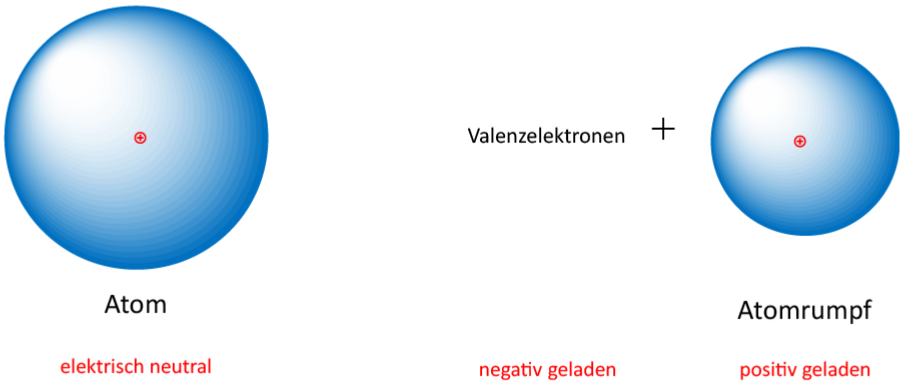
Elektronegativitäten von Aluminium, Sauerstoff und Fluor

Aluminium	Sauerstoff	Fluor
EN = 1,5	EN = 3,5	EN = 4,0

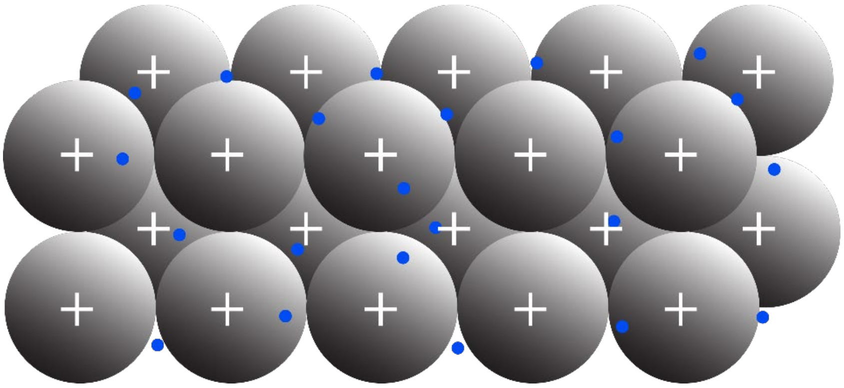
Wir haben im ersten Kapitel die Elektronegativität folgendermassen definiert:

Die Elektronegativität (EN) ist ein relatives Mass dafür, wie stark Elektronen von einem Atom angezogen werden.

Die tiefe Elektronegativität lässt die Vorstellung als plausibel erscheinen, dass die Valenzelektronen ihren Platz verlassen können und nicht fest bei nur einem Aluminiumatom bleiben. Wenn wir dem Aluminiumatom formal die Valenzelektronen entziehen, entstehen natürlich **Atomrümpfe**, die zurückbleiben. Bei Metallen spricht man deshalb von den frei beweglichen Valenzelektronen und Atomrümpfen.



Die frei beweglichen Elektronen, welche bisweilen als ***Elektronengas*** bezeichnet werden, halten die übrigbleibenden positiv geladenen Atomrümpfe zusammen.

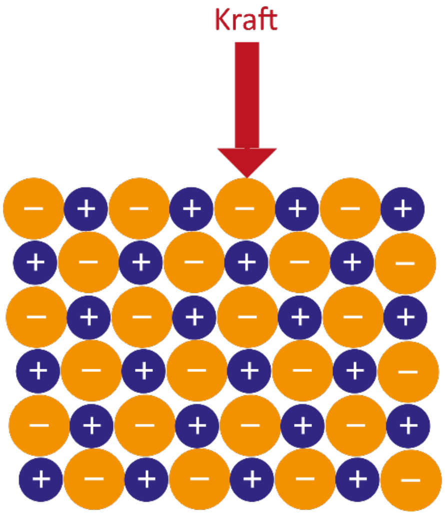


In der Räuber/Opfer-Analogie können wir sagen, dass die Elektronenopfer sich ihre Valenzelektronen nicht streitig machen, sondern untereinander teilen.

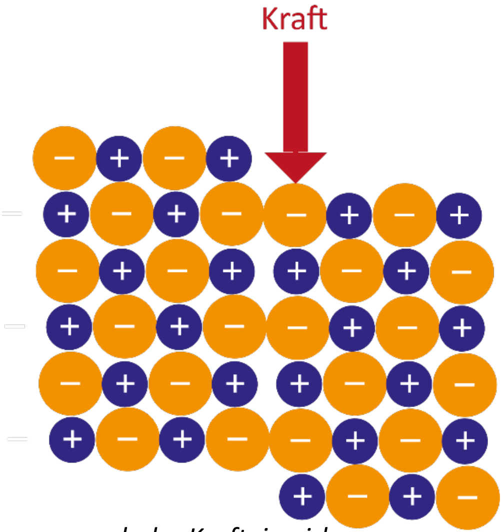
Anmerkung: Es ist wichtig zu wissen, dass die Aluminiumatome in einem metallischen Feststoff zwar formal zu Atomrümpfen werden, sich aber im Durchschnitt weiterhin drei Valenzelektronen bei jedem Aluminiumrumpf aufhalten, wenn auch nicht immer dieselben. Diese Situation ist deutlich zu unterscheiden von Aluminiumkationen Al^{3+} in einer ionischen Verbindung, bei welchen die Valenzelektronen entrissen wurden und keine Valenzelektronen aufzufinden sind.

Arbeitsblatt III/1: Ionenbindung und metallische Bindung im Vergleich

Auftrag 1: Überlegen Sie sich, welche Folgen eine Verschiebung der Ionen für den Zusammenhalt der Ionen haben wird.

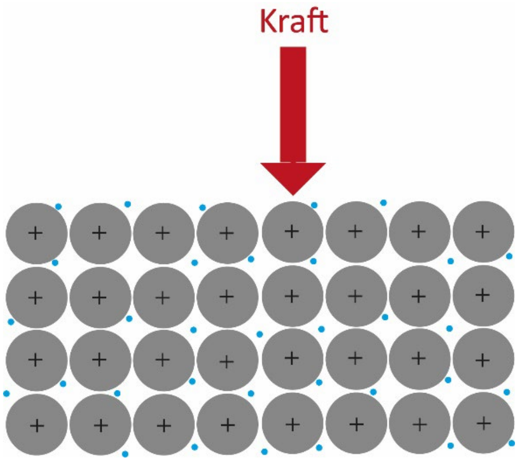


Vor der Krafteinwirkung

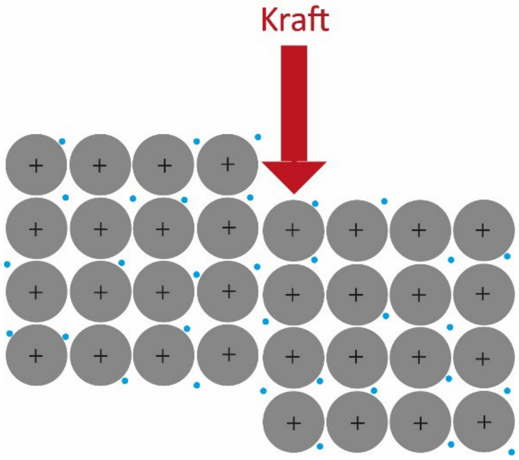


nach der Krafteinwirkung

Auftrag 2: Überlegen Sie sich, welche Folgen eine Verschiebung der Atomrümpfe haben wird für den Zusammenhalt der Atomrümpfe.



Vor der Krafteinwirkung



nach der Krafteinwirkung

3.4 Vergleich der bisher erörterten Bindungsarten

Nachdem wir die beiden Bindungsarten «Ionenbindung» und «metallische Bindung» erörtert haben, ist es sinnvoll, die beiden Bindungsarten miteinander zu vergleichen.

Wir können zuerst repetieren, welche Kräfte in einem Ionengitter und einem metallischen Gitter zwischen den Teilchen wirken.

Ionenbindung: Zwischen ungleich geladenen Ionen wirken Anziehungskräfte, zwischen den gleich geladenen Ionen wirken Abstossungskräfte.

Metallische Bindung: Zwischen den positiv geladenen Atomrümpfen wirken Abstossungskräfte, zwischen den positiv geladenen Atomrümpfen und den frei beweglichen Elektronen wirken Anziehungskräfte.

Üben wir Kraft auf ein Stück eines salzartigen Stoffes oder auf einen Stück Metall aus, so kann dies eine Verschiebung der Teilchen in der Gitteranordnung zur Folge haben. Die nächste Überlegung betrifft die Folgen, welche so eine Verschiebung der Teilchen in beiden Fällen haben kann.

Ionenbindung: Jede Verschiebung der Ionen in einem Ionenkristall wird die gleich geladenen Ionen näher zueinander bringen. Dies bringt eine Schwächung oder sogar den Zerfall der Gitterstruktur mit sich.

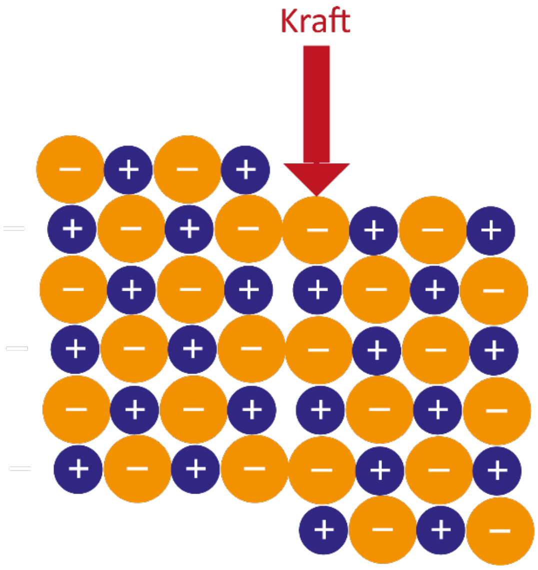


Abb. 1 Erklärung der Sprödheit von Salzen

Auf diese Weise können wir die Sprödheit der Salze verstehen.

Metallische Bindung: Eine Verschiebung der Atomrümpfe wird keine gravierenden Konsequenzen für die Stabilität des Gitters haben, da die Elektronen im Gitter frei beweglich sind und die Lage der positiv geladenen Atomrümpfe somit keine grosse Rolle spielt.

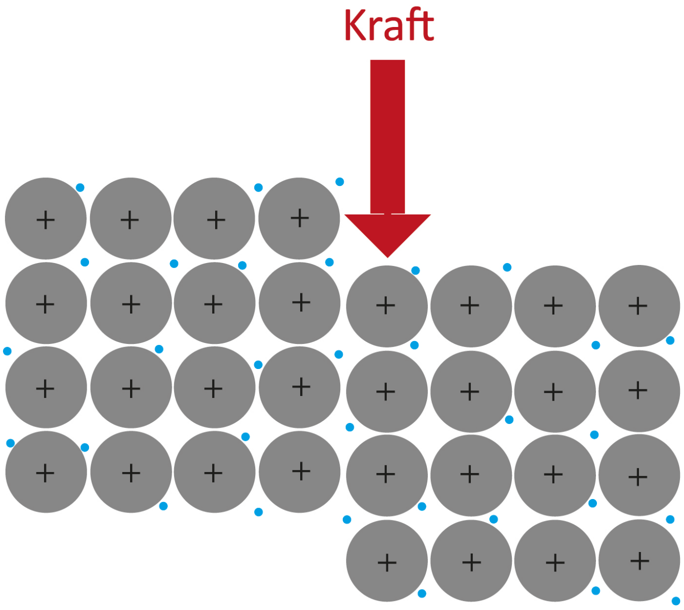


Abb. 2 Erklärung der Verformbarkeit von Metallen

Diese Überlegung ermöglicht es uns zu verstehen, weshalb die Metalle so gut verformbar (duktil) sind.

Aluminium kann beispielsweise zu einer Folie mit der Dicke von Bruchteilen von Millimetern auswalzen. Die Folie ist biegsam und gut verformbar.

Abb. 4 verformbare Aluminiumfolie

Arbeitsblatt III/2: Selbsterklärungsaufgaben zur Vertiefung

Auftrag 1: Aluminiumoxid (Al_2O_3) ist ein Salz. Aluminium als Reinstoff ist ein metallischer Stoff.

a) Hugo behauptet aber, dass in beiden Verbindungen die Metallatome als die exakt gleichen Al^{3+}-Kationen vorliegen. Erklären Sie ihm, was an seiner Überlegung nicht stimmt und wieso es falsch ist, bei metallischen Verbindungen von Kationen zu sprechen.

Auftrag 2: Hugo behauptet ausserdem, dass die Metallatome in einer metallischen Verbindung durch das Metallgitter zusammengehalten werden. Erklären Sie ihm, was der wirkliche Grund dafür ist, dass Metalle bei Raumtemperatur typischerweise fest sind und die Metallatome zusammengehalten werden. Fertigen Sie hierzu eine Skizze an.

Auftrag 3: Hugo ist zudem der Meinung, dass metallische Stoffe Salze sind, welche nur aus positiven Ionen (Kationen) aufgebaut sind.

a) Warum wäre eine solche Verbindung komplett instabil?

b) Zählen Sie die Gemeinsamkeiten sowie die Unterschiede zwischen Salzen und Metallen auf, um ihm aufzuzeigen, dass es Sinn macht, Salze von Metallen abzugrenzen.

Gemeinsamkeiten

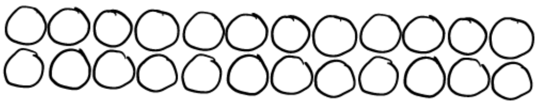
Unterschiede	**Ionische Verbindungen (Salze)**	**Metallische Verbindungen (Metalle)**
Art der enthaltenen Elemente (Metalle M, Nichtmetalle NM)		
Aufgebaut aus…		
Lokalisierung/Beweglichkeit der Valenzelektronen		
Zusammenhalt der Teilchen wegen…		
Leiten des elektrischen Stroms		
Verformbarkeit / Duktilität		

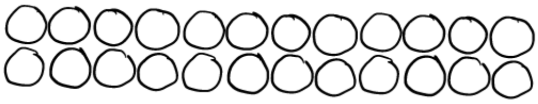
Auftrag 4: Erklären Sie die unterschiedlichen elektrischen Leitfähigkeiten der aufgeführten Stoffe. Ein höherer Wert entspricht einer grösseren elektrischen Leitfähigkeit.

	Natriumchlorid (NaCl)	**Aluminium (Al)**	**Natrium (Na)**
elektrische Leitfähigkeit bei Raumtemperatur	keine Leitfähigkeit	$37 * 10^6$ A / V m	$21 * 10^6$ A / V m

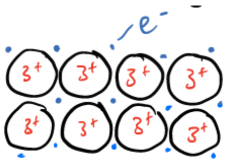
3.5 Eigenschaften von Metallen

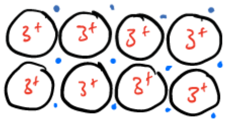
3.5.1 Wärmeleitfähigkeit





3.5.2 Elektrische Leitfähigkeit





3.5.3 Duktilität

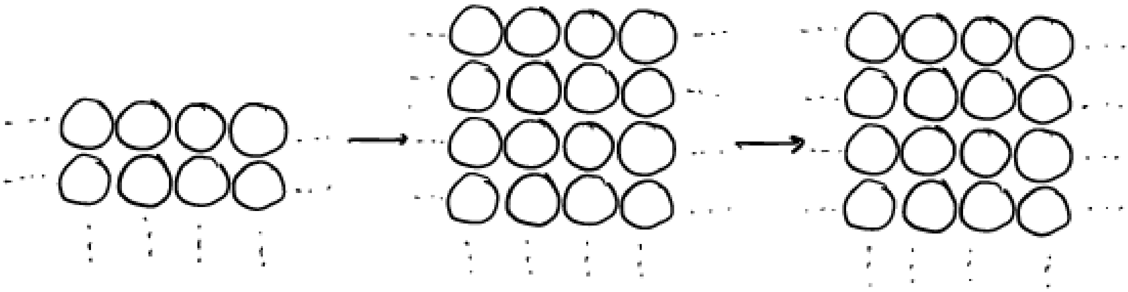
Arbeitsblatt III/3: Eigenschaften metallischer Stoffe

Auftrag 1: Im Gegensatz zu Salzen seien alle Metalle hart und durch mechanische Kraftanwendung nicht zu spalten behauptet Hugo. Ein Zentimeter dickes Natriumstück ist aber leicht mit einem Küchenmesser zu durchschneiden. Ein Stück Aluminiumblech ist hingegen mit einem Messer nicht zu durchschneiden. Erklären Sie diesen Umstand.

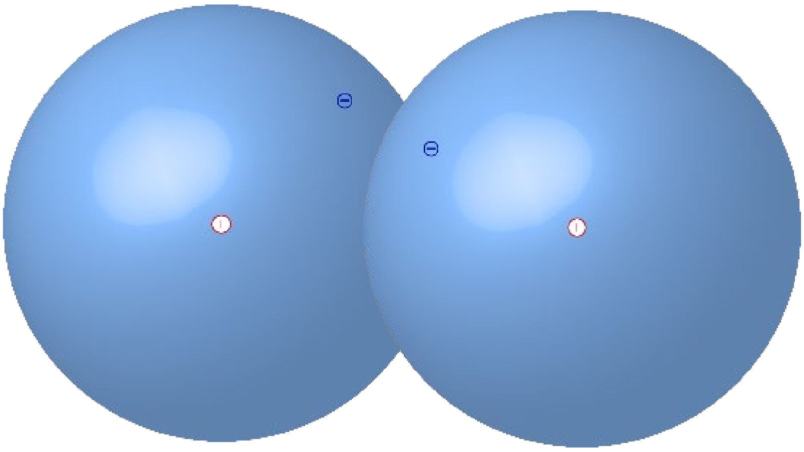
Auftrag 2: Wird ein Stück Metall an der einen Seite erhitzt, wird die Wärme schnell auf die andere Seite übertragen. Was ist der Grund für die gute Wärmeleitfähigkeit von Metallen?

Auftrag 3: Wenn man ein Aluminiumblech mit einem Bunsenbrenner erhitzt, sinkt die elektrische Leitfähigkeit. Können Sie dieses Phänomen anhand des Elektronengasmodells erklären?

3.6 Legierungen



IV. Kovalente Bindung



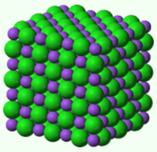
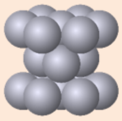
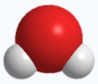
4.1 Ergebnisse der Versuche zur Leitfähigkeit verschiedener Stoffe:

Stoff	*Natriumchlorid (Kochsalzkristall)*	*Aluminiumblech*	*Eis (fest)*	*reines Wasser (flüssig)*
elektrische Leitfähigkeit				
frei bewegliche Teilchen (Ja/nein)				

4.1.1 Folgerungen

Sie sind hier

4.2 Übersicht

Bindungsart	ionische Bindung	metallische Bindung	kovalente Bindung		
Art der Elemente	Metalle und Nichtmetalle	Metalle unter sich	Nichtmetalle unter sich		
Anziehung zwischen	Anionen und Kationen	Atomrümpfen + Elektronengas	Atomrümpfen + Elektronen		
Art der Teilchen oder Verbände	riesiger Ionenverband, Anordnung gemäss Ionengitter	riesiger Atomverband, Anordnung gemäss Metallgitter	kleine Moleküle		
Stoffklasse					
Abbildungen					

4.3 Aggregatzustand von Stoffen aufgebaut aus Nichtmetallen

Betrachtet man alle nichtmetallischen Elemente, so besitzen die Atome von Wasserstoff den einfachsten Aufbau. Ein Stoff der nur aus dem Element Wasserstoff (H) aufgebaut ist (ein sogenannter Elementarstoff) existiert. Wie liegt dieser Stoff bei Raumtemperatur vor?

Stoff	*Natriumchlorid*	*Aluminiumblech*	*reines Wasser*	*Wasserstoff*
Aggregatzustand bei Raumtemperatur				
Schmelzpunkt				

4.3.1 Folgerungen

Arbeitsblatt IV/1: Einführungsexperimente zur kovalenten Bindung

Auftrag 1: Welches Experiment zeigt auf, dass Wasser als Stoff nicht als Salz, bestehend aus Ionen, vorliegen kann?

Auftrag 2: Welches Ergebnis der vorgeführten Experimente mit dem Stoff Wasser müsste anders ausfallen, würde dieser Stoff mittels metallischer Bindung zusammengehalten werden?

Auftrag 3: In den beiden vorhergehenden Kapiteln «Ionenbindung» und «metallische Bindung» haben Sie gelernt, dass Salze und Metalle relativ hohe Schmelz- und Siedepunkte haben. Können Sie diese Tatsache erklären?

Auftrag 4: Im Unterricht hat Ihnen Ihre Lehrkraft aufgezeigt, dass Wasserstoff bei Zimmertemperatur gasförmig ist und einen Siedepunkt von – 252,9 °C aufweist. Welche Aussagen über die Beschaffenheit der kleinsten Teilchen, aus denen Wasserstoff besteht, können Sie aufgrund der obigen Tatsachen machen? Äussern Sie sich auch zu der Stärke der Kräfte, welche zwischen diesen Teilchen wirken.

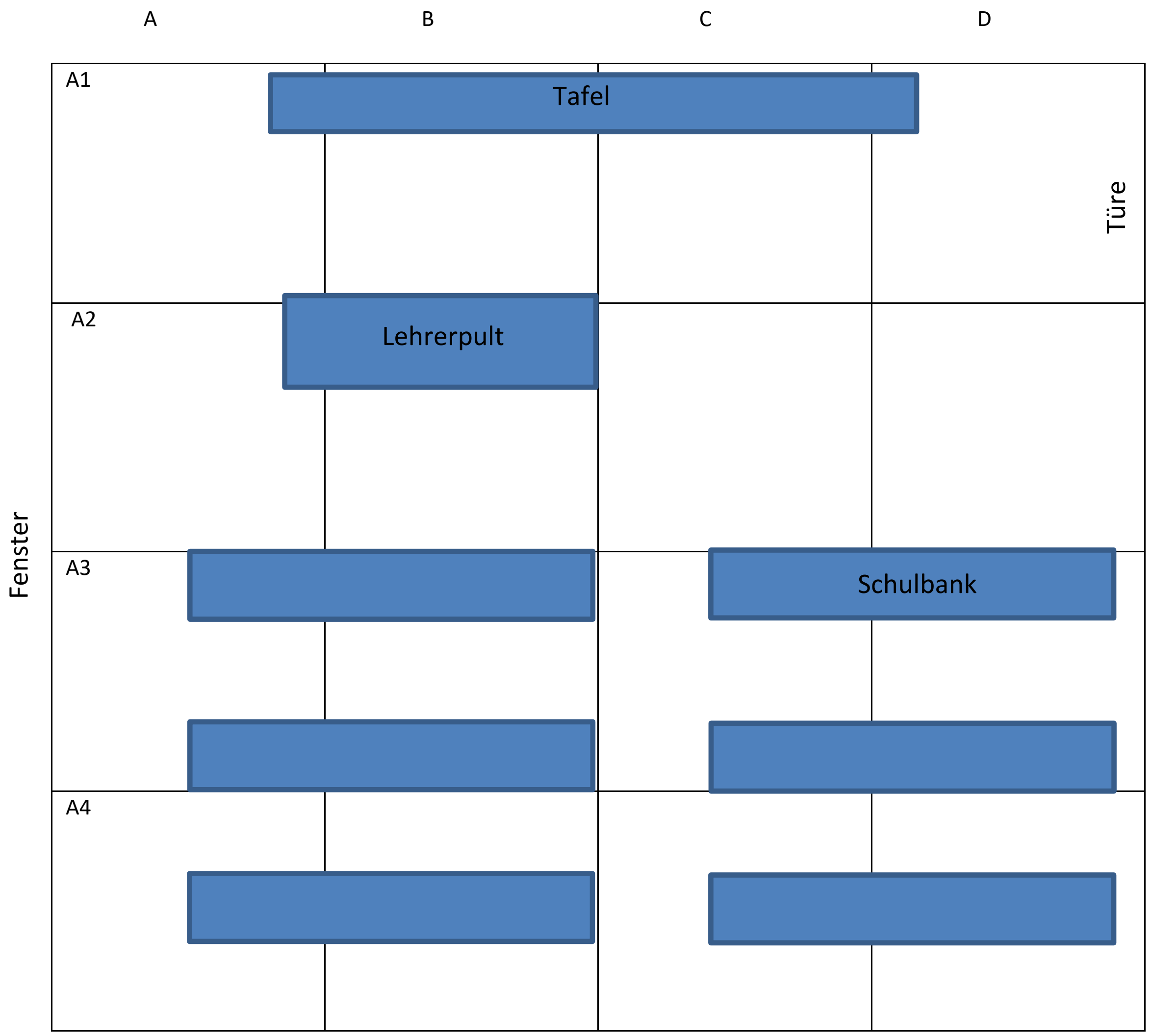
Arbeitsblatt IV/2: Wasserstoffatom

Auftrag 1: Dimensionen des Wasserstoffatoms:

Atomradius des H-Atoms:	52'920 fm (10^{-15} m)
Atomkern-Durchmesser von einem H-Atom:	1.757 fm (10^{-15} m)

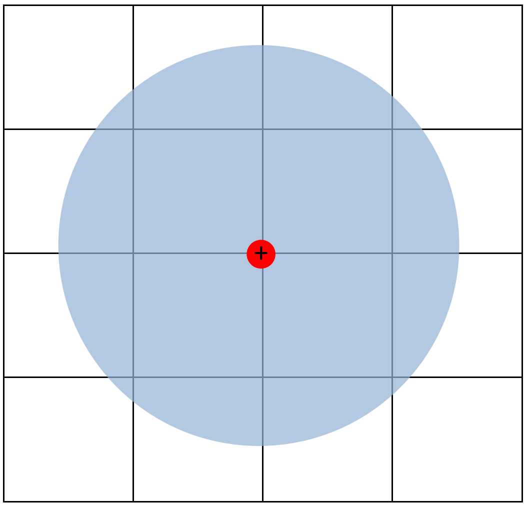
Angenommen, der **Atomkern** eines vergrösserten Wasserstoffatoms hätte den Durchmesser von 1 cm, wie viele Meter müssten Sie sich vom Kern entfernen bis Sie das Atom «verlassen» würden?

Auftrag 2: Angenommen, Sie stehen vor der Türe eines Schulzimmers und wissen, dass eine Lehrperson gerade unterrichtet, ohne aber in das Schulzimmer blicken zu können. Wo würden Sie die Lehrperson am ehesten erwarten? Markieren Sie Flächen mit roter Farbe, auf welchen sich die Lehrperson mit hoher Wahrscheinlichkeit befindet.



Auftrag 3: Wo würden Sie tendenziell eher erwarten ein Elektron in einem Wasserstoffatom anzutreffen und wo weniger? Welche der vier Varianten erachten sie als realistisch und welche weniger. Begründen Sie auch wieso sie die Varianten ihrer Meinung nach nicht realistisch sind.

A



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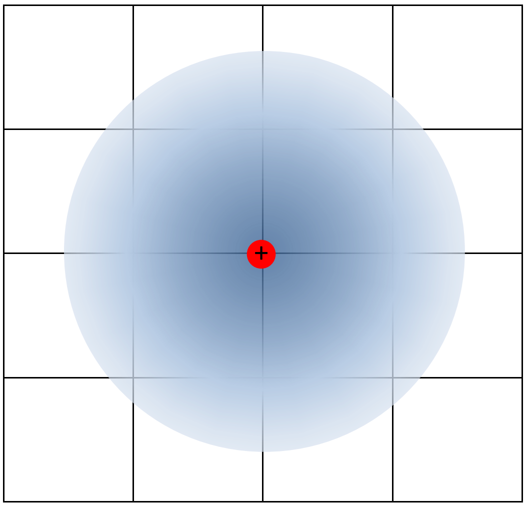

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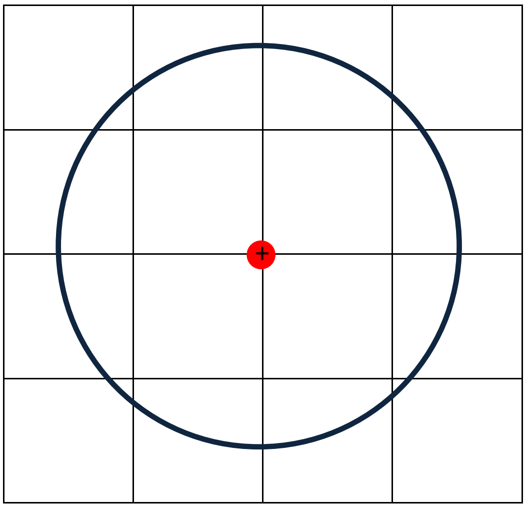

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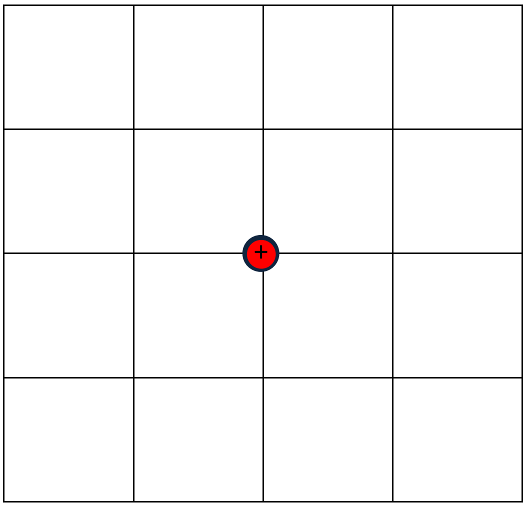


A:

B:

C:

D:

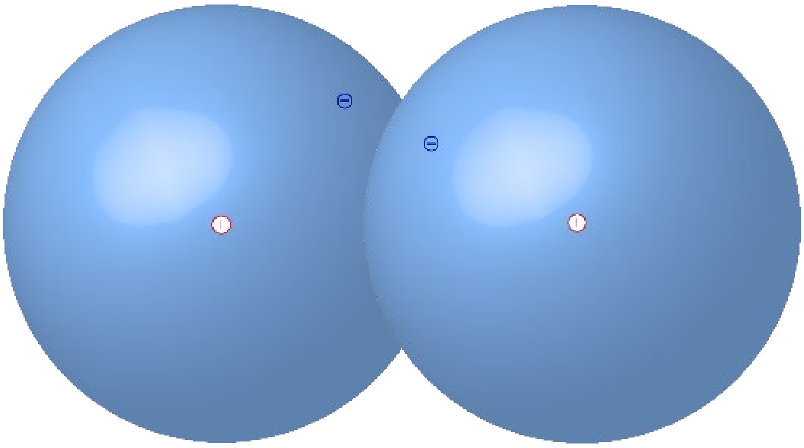
4.4 Von Schalen zu Elektronenwolken

Das Bohr'sche Schalenmodell erklärt für einzelne Atome bereits einige Sachverhalte (Atomflammenfarben, Ionisierungsenergien). Das Elektronenschalenmodell gerät aber bei der Beschreibung von Molekülen an seine Grenzen und kann chemische Bindungen nicht erklären. Es wiederspricht zudem moderneren quantenmechanischen Ansichten, dass sich ein Elektron nicht beliebig genau beschreiben lässt (Heisenberg'sche Unschärferelation). Das Bild von Elektronenbahnen wird dadurch ersetzt, dass Elektronen nur **bestimmte Aufenthaltswahrscheinlichkeiten** zugesprochen werden.

Definition: Elektronenwolke

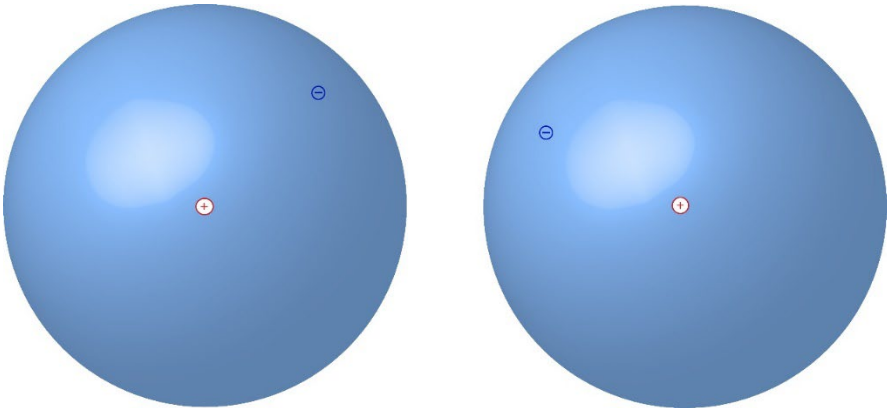
Das Modell mit Elektronenwolken hat den Vorteil, dass diese «verformbar» sind und entsprechend auf weitere Atomkerne «reagieren» können. Die Wahrscheinlichkeit ein Elektron an einem bestimmten Ort anzutreffen ändert sich mit dem Hinzufügen weiterer Atomkerne und Elektronen. Mit diesem Modell lässt sich die kovalente Bindung besser beschreiben.

4.5 H_2-Molekül

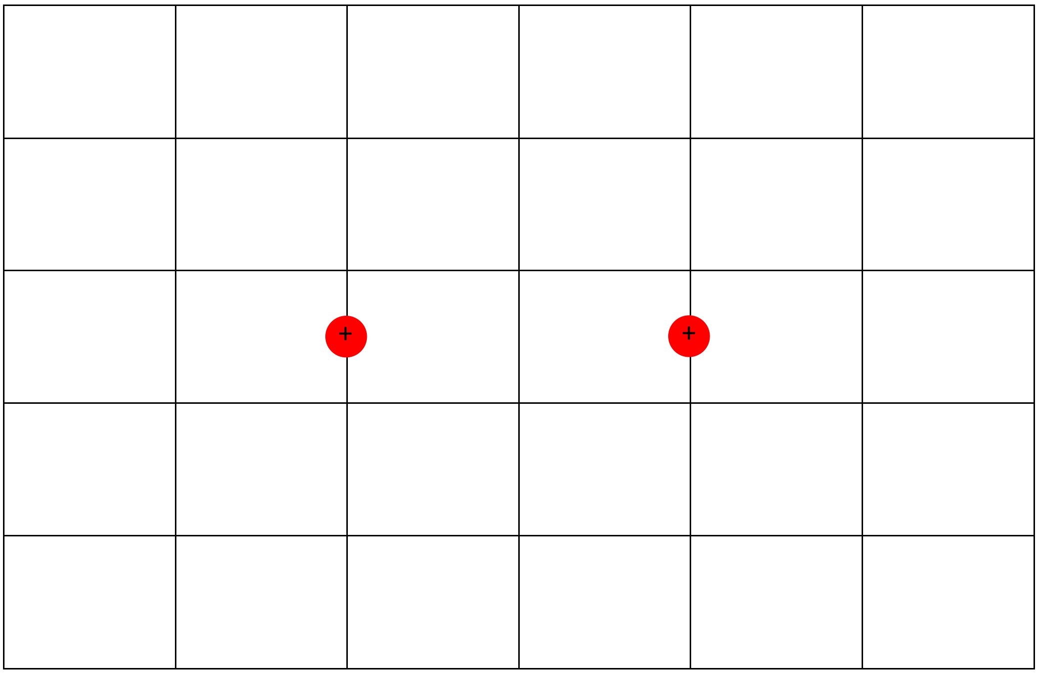


Arbeitsblatt IV/3: Zwei Wasserstoffatome

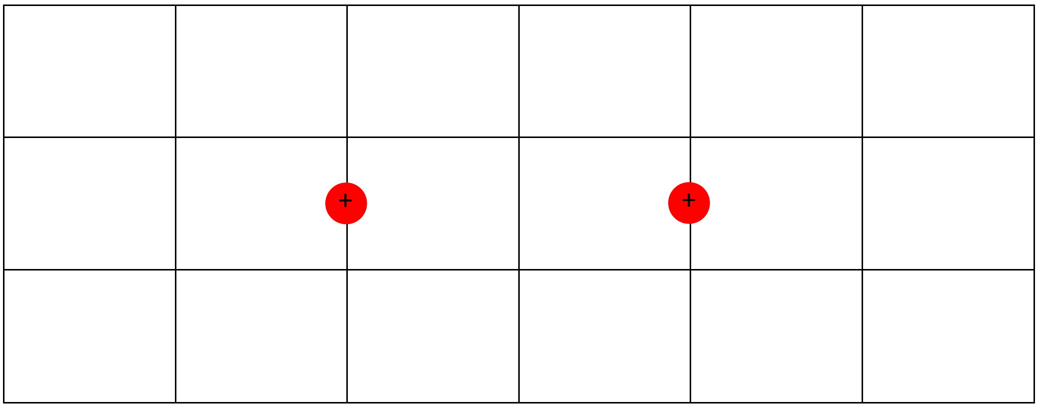
Auftrag 1: Verbinden Sie, diejenigen elektrisch geladenen Teilchen der beiden Wasserstoffatome, welche sich anziehen und verwenden Sie dazu eine grüne Farbe. Verbinden Sie in einem zweiten Schritt sich abstossende, geladene Teilchen mit einer roten Farbe.



Auftrag 2: Wo würden Sie tendenziell eher erwarten Elektronen in einem Wasserstoffmolekül (H_2-Molekül) anzutreffen und wo weniger? Zeichnen Sie eine Fläche ein, in welchem Sie eine hohe Wahrscheinlichkeit erwarten ein Elektron zu finden.

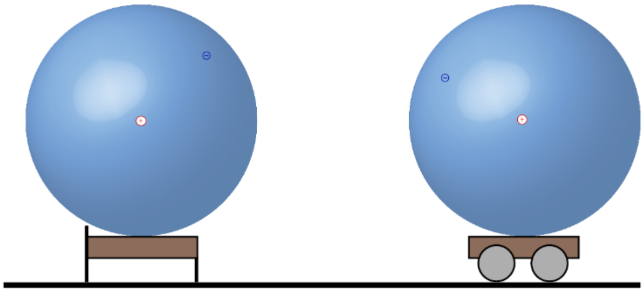
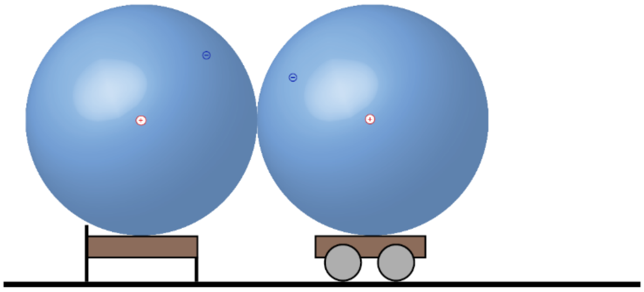
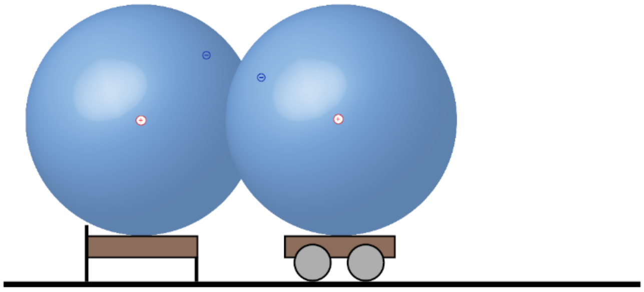
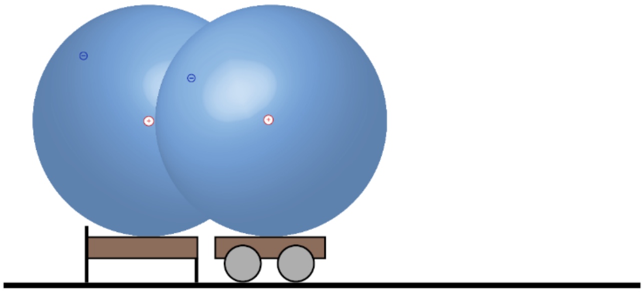


4.5.1 Aufenthaltswahrscheinlichkeit bei H_2



4.5.2 Lewis-Schreibweise

4.5.3 Zwei sich nähernde Wasserstoffatome - Zuganalogie

	Abstossung der Elektronenhüllen	Anziehung der Elektronen und Atomkerne	Abstossung der Atomkerne
	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant
	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant
	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant
	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant	☐ klein ☐ mittel ☐ gross ☐ sehr gross ☐ dominant

Arbeitsblatt IV/4: Das Wasserstoffmolekül (H_2)

Auftrag 1: Hugo argumentiert, dass gemäss dem Coulombgesetz sich positive und negative Ladung je mehr anziehen, desto näher diese sich sind. Er ist deshalb der Meinung, dass die zwei Wasserstoffatome sich möglichst nahekommen müssen. Erkläre ihm in vollständigen Sätzen, wieso die zwei Wasserstoffatome in einem H_2-Molekül nicht beliebig nahe beieinander anzutreffen sind.

Auftrag 2: Erkläre, wieso man Energie aufwenden muss, um ein Wasserstoffmolekül in seine einzelnen Wasserstoffatome zu zerlegen.

Auftrag 3: Was ist der Grund dafür, dass zwei Wasserstoffatome in einem H_2-Molekül zusammengehalten werden?

Arbeitsblatt IV/5: Moleküle mit Wasserstoff

Auftrag 1: Machen Sie einen Vorschlag zum Aufbau eines Moleküls, bestehend aus möglichst vielen **H-Atomen** und …

a) … einem **Kohlenstoffatom** (C)

b) … einem **Stickstoffatom** (N).

c) … einem **Sauerstoffatom** (O).

d) … einem **Fluoratom** (F).

e) … einem **Neonatom** (Ne).

Arbeitsblatt IV/6: Herleiten von Molekülformeln

Auftrag 1: Zeichne für die folgenden Stoffe die Lewisformeln. Welche Verbindung entsteht aus…

a) Einem C-Atom und 4 F-Atomen?

b) Aus zwei F und einem O-Atom?

c) Einem H- und einem Cl-Atom?

d) Einem K-Atom und einem Cl-Atom?

e) Aus einem N-Atom und Cl-Atomen?

f) Aus einem Mg- und O-atom

Aufgabe 2: Hugo behauptet HCl und KCl sind sich strukturell sehr ähnlich und man könne bei HCl-Molekülen einfach das H-Atom durch ein K-Atome ersetzten. Erkläre ihm, wie sich die beiden Stoffe voneinander unterscheiden.

Aufgabe 3: Zeichne folgende Moleküle

a) O_2

b) N_2

c) CS_2

d) CO_2

4.6 Definition eines Moleküls

Definition:

Ein ***Molekül*** ist ein Atomverband aus mindestens zwei nichtmetallischen Atomen, welche über kovalente Bindungen miteinander verknüpft sind.

Auftrag 1: Setzen Sie Häkchen (✓) falls korrekt oder Kreuze (**x**), falls nicht korrekt.

Summenformel	ausschliesslich nichtmetallische Atome	kovalente Bindung(en)	ungeladene Atome (keine Ionen)	mindestens zwei Atome	Falls kein Molekül: korrekter Begriff
H_2					
NaCl					
Ar					
H_2O					
CuZn					
LiF					
Fe					

4.7 Verhältnisformel vs. Strukturformel oder Molekülformel

Im Chemieunterricht treffen Sie häufig auf chemische Formeln. Die Aussagekraft der Formel ist aber für Salze und Metalle nicht die gleiche wie für Moleküle:

Chemische Formel	HCl	NaCl	NaK
Bindungstyp:			
Vorliegen der kleinsten Teilchen:			Atomrümpfe und Elektronengas
Bezeichnung:	Molekül		
Verhältnis der enthaltenen Elemente:	1 H-Atom : 1 Cl-Atom		

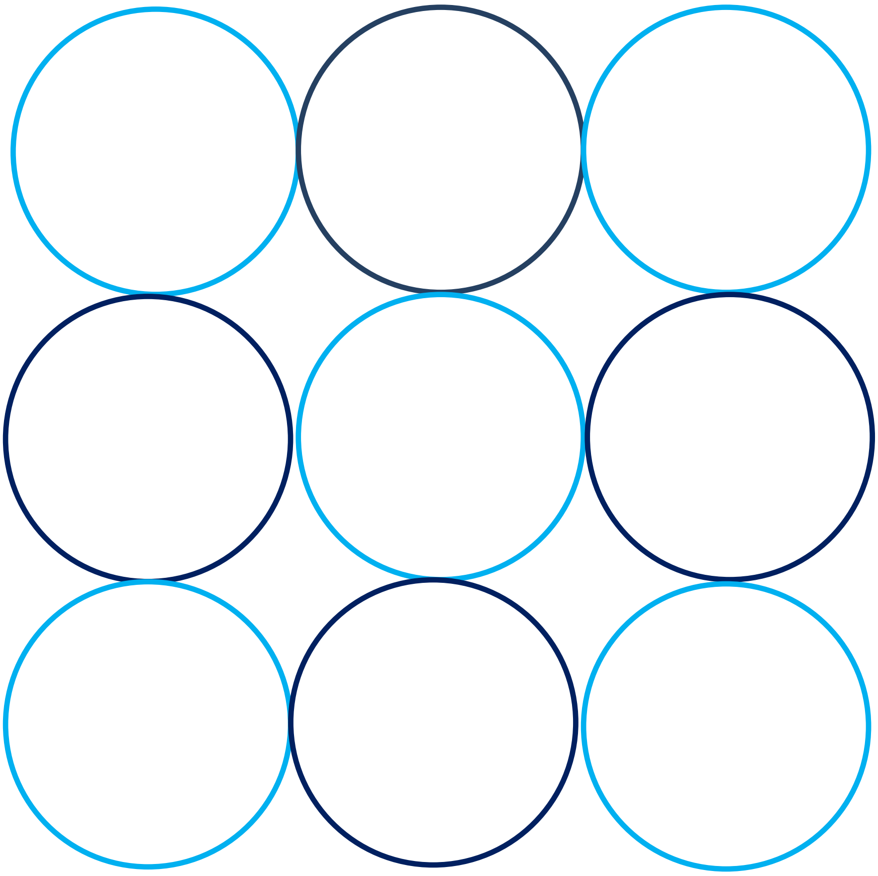
Fazit:

4.8 Mehratomige Ionen – Molekül-Ionen

Experiment: NH_4Cl

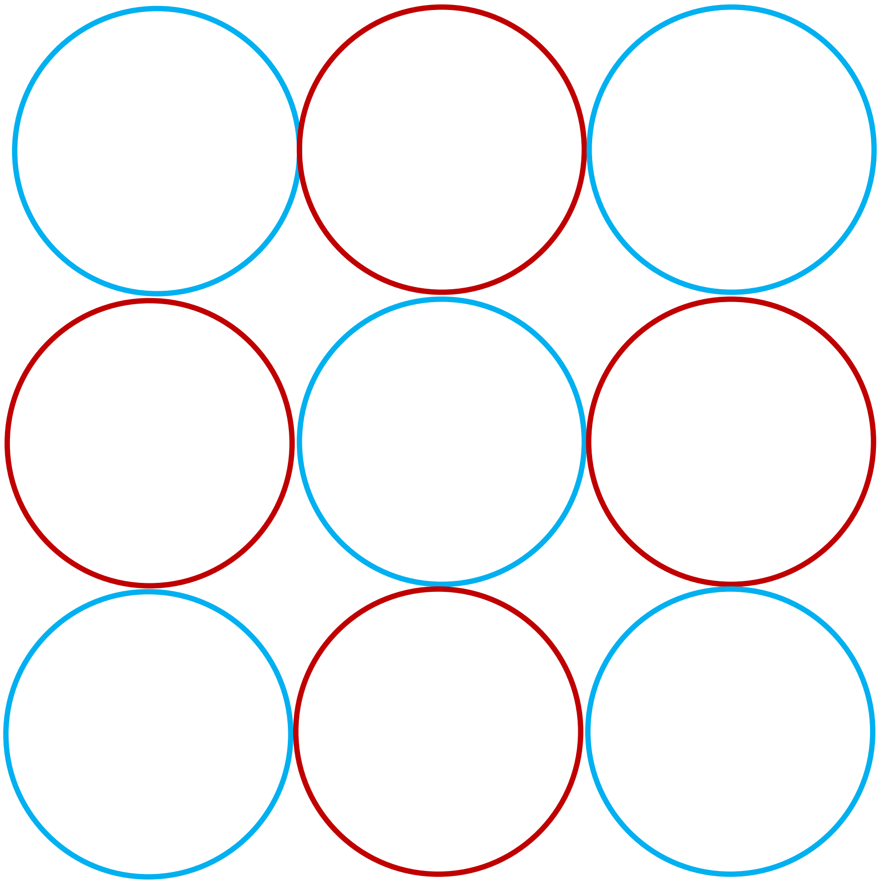
Eigenschaften:

Aufgabe 1: Zeichne NH_3 in der Lewis-Schreibweise.



Experiment:

Auftrag 2: Folgende Abbildung illustriert Kalziumcarbonat ($CaCO_3$). Aus welchen Ionen besteht die Verbindung? Welches sind die Ladungen, die sie erwarten bei den Ionen?



4.8.1 Salze mit Molekülionen

Die mehratomigen Ionen entstehen vorwiegend durch Reaktion von Säuren und Basen, ihre Namen leiten sich deshalb aus den Namen der entsprechenden Säuren und Basen ab. Da das Kapitel «Säure-Base-Reaktionen» erst wesentlich später im Chemieunterricht ansteht, werden hier die Namen und Formeln einiger wichtiger Ionen einfach angeben. Die Entstehung dieser Ionen wird erst später im Unterricht wesentlich genauer zur Sprache kommen. Wichtig ist, dass die Molekül-Ionen als Ganzes eine Ladung tragen.

4.8.2 Wichtigste Molekül-Anionen

Hydroxid	$(OH)^-$
Nitrat-Ion	$(NO_3)^-$
Hydrogencarbonat-Ion	$(HCO_3)^-$
Carbonat-Ion	$(CO_3)^{2-}$
Sulfat-Ion	$(SO_4)^{2-}$
Phosphat-Ion	$(PO_4)^{3-}$

4.8.3 Wichtigstes Molekül-Kation

Ammonium-Ion	$(NH_4)^+$

Arbeitsblatt IV/7: Molekül-Ionen

Auftrag 1: Füllen Sie die untenstehende Tabelle aus.

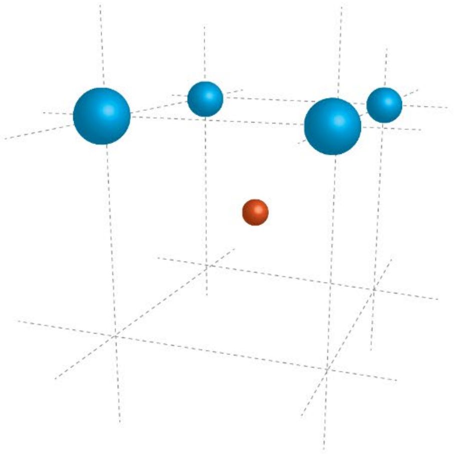
Verhältnisformel des Salzes	Name des Salzes	Formel des Kations	Formel des Anions
		Na^+	$(CO_3)^{2-}$
	Kalziumhydroxid		
NH_4NO_3			
		Fe^{3+}	O^{2-}
	Kupfer(II)-sulfat		
	Ammoniumsulfid		
	Kalziumnitrat		
	Natriumhydrogen-carbonat		
	Aluminiumsulfat		

Auftrag 2: NH_4NO_3 besteht nur aus Nichtmetallen, dennoch ist es falsch von einem Molekül zu sprechen. Erklären Sie wieso dies der Fall ist.

Arbeitsblatt IV/8: Anordnung der Elektronenwolken im Raum

Welches ist Ihrer Meinung die beste räumliche Anordnung, wenn vier doppelt besetzte Elektronenwolken um ein Zentralatom angeordnet werden? Begründen Sie Ihre Wahl.

A



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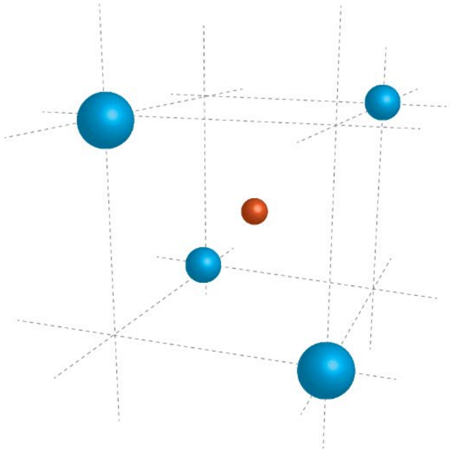

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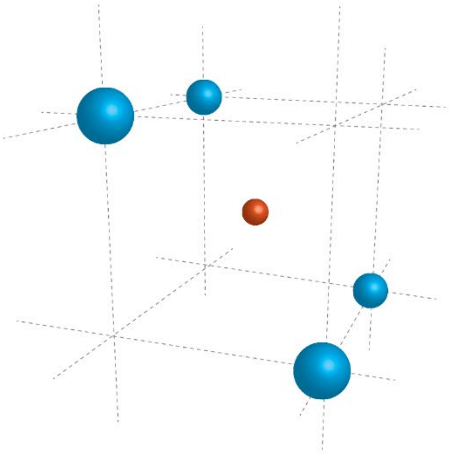

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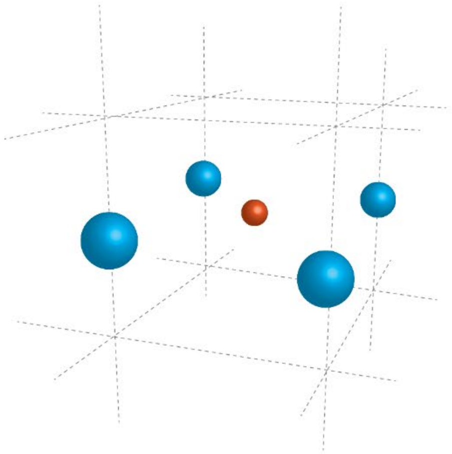

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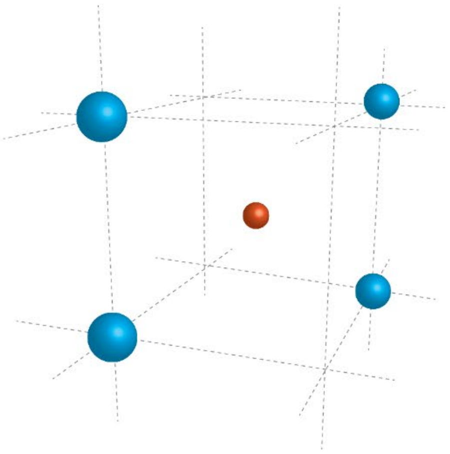

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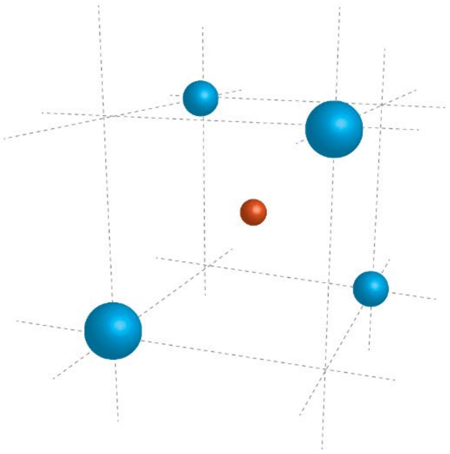


4.9 räumliche Anordnung der Elektronenwolken

Die gegenseitige Abstossung der Elektronenwolken ist der Grund für die räumliche Anordnung der Atome um ein Zentralatom. Das entsprechende Modell wird deshalb auch als ***Elektronenpaarabstossungs-Modell (EPA-Modell)*** bezeichnet.

Die räumliche Gestalt von Molekülen wird durch die gegenseitige Abstossung der (bindenden und nichtbindenden) Elektronenwolken bestimmt.

lineare Gestalt 180°

Bsp: Kohlenstoffdioxid CO_2

Räumliche Umgebung **linear (gestreckt)**

Bindungswinkel ∠O-C-O **180°**

planar trigonale Gestalt – ebenes Dreieck ~120°

Bsp: Methanal CH_2O

Räumliche Umgebung **trigonal-planar (Dreiecksebene)**

Bindungswinkel ∠O-C-H ~**120°**

tetraedrische Gestalt 109.5°

Bsp: Methan CH_4

Räumliche Umgebung **tetraedrisch**

Bindungswinkel ∠H-C-H ~**109°**

4.8.1 Verfahren zur Bestimmung der räumlichen Gestalt von Molekülen

1) Ausgangspunkt der Ermittlung ist die Lewisformel des betreffenden Moleküls.
2) Gesamtanzahl der Elektronenwolken um das Zentralatom wird ermittelt (bindende **und** nichtbindende Wolken).
   - Mehrfachbindungen zählen als eine Wolke.
3) Die Anordnung der Wolken wird ermittelt:

   4 Wolken → tetraedrische Gestalt
   3 Wolken → planar trigonale Gestalt (ebenes Dreieck)
   2 Wolken → lineare Gestalt

4) Die bindenden Wolken ergeben nun die räumliche Gestalt des Moleküls.

Arbeitsblatt IV/9: Moleküle - Repetition und räumliche Anordnung

Die folgenden Moleküle haben Sie teilweise bereits gezeichnet. Bestimmen Sie die räumliche Anordnung um das **Zentralatom** (fett).

Auftrag 1: Zeichnen Sie für die folgenden Stoffe die Lewis-Formeln. Welche Verbindung entsteht aus …

f) **C**F_4

g) F_2**O**

h) H**Cl**

i) K**Cl**

j) **N**Cl_3

k) Mg**O**

Aufgabe 2: Zeichnen Sie folgende Moleküle:

a) **O_2**

b) **N_2**

c) **C**S_2

d) **C**O_2

Auftrag 3: Zeichnen Sie für die folgenden Stoffe die Lewis-Formeln. Welche Verbindung entsteht aus …

a) **Cl**$_2$?

b) 1 **N**-Atom und Br-Atomen?

c) **C**H$_4$O?

d) 2 H- und 2 **N**-Atomen?

e) **C**H$_2$O?

f) **Li**H?

g) **C**$_2$H$_2$?

h) CaCl$_2$?

i) **B**F$_3$

Zusatzaufgaben zum Herleiten von Molekülformeln

Auftrag 1: Zeichne für die folgenden Stoffe die Lewisformeln. Welche Verbindung entsteht aus …

a) Cl-Atomen?

b) 1 N-Atom und Br-Atomen?

c) CH_4O?

d) 2 H- und 2 N-Atomen?

e) CH_2O?

f) LiH?

g) C_2H_2?

h) $CaCl_2$?

Bonus: S_8 (**Tipp:** keine Doppel- und Dreifachbindungen)

4.10 Zusammenfassung

Leitfähigkeit und generelle Eigenschaften

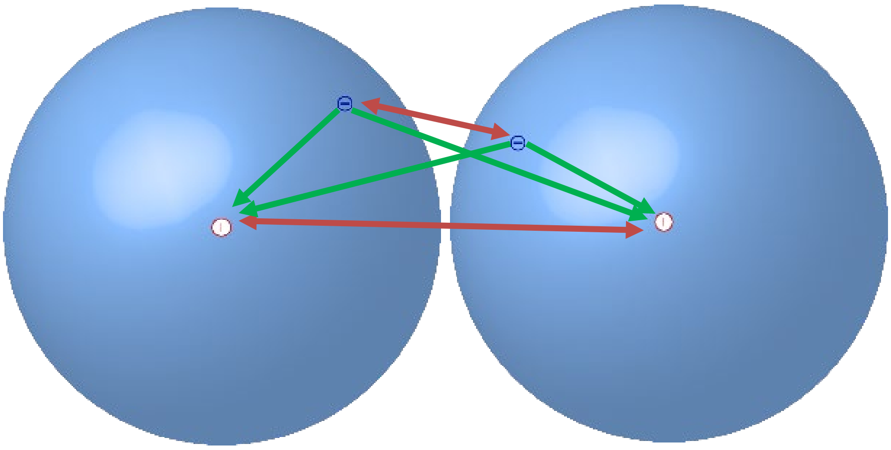
Stoffe mit molekularem Aufbau enthalten nur nichtmetallische Elemente. Sie unterscheiden sich generell von Salzen und Metallen, die typischerweise bei Raumtemperatur als Feststoffe vorliegen. Dies liegt daran, dass bei Stoffen, die aus Nichtmetallen aufgebaut sind, sich auch kleinere stabilere «Einheiten» bilden können. Diese werden als *Moleküle* bezeichnet. Die Anziehungskräfte zwischen diesen Molekülen («zwischenmolekulare Kräfte → nächstes Kapitel) müssen deutlich geringer sein als die Anziehungskräfte zwischen den Ionen bei Salzen und den Atomrümpfen und dem Elektronengas bei Metallen. Dies heisst aber nicht, dass kovalente Bindungen an sich schwächer sind: Die Anziehungskräfte innerhalb eines Moleküls sind ebenfalls stark, wenn kovalente Bindungen in einem Molekül vorkommen. Zudem sind Moleküle unter normalen Umständen neutrale Teilchen. Molekulare Reinstoffe leiten den elektrischen Strom deshalb nicht.

Schalen und Elektronenwolken

Ein Modell der Atome mit Elektronen auf fixen Elektronenbahnen wird ergänzt durch ein Modell, in dem Elektronen nur bestimmte *Aufenthaltswahrscheinlichkeiten* an verschiedenen Orten zugesprochen werden. Dazu ist das Modell der *Elektronenwolke* hilfreich: Eine Elektronenwolke beschreibt einen Raum, in welchem eine grosse Wahrscheinlichkeit herrscht, das Elektron anzutreffen.

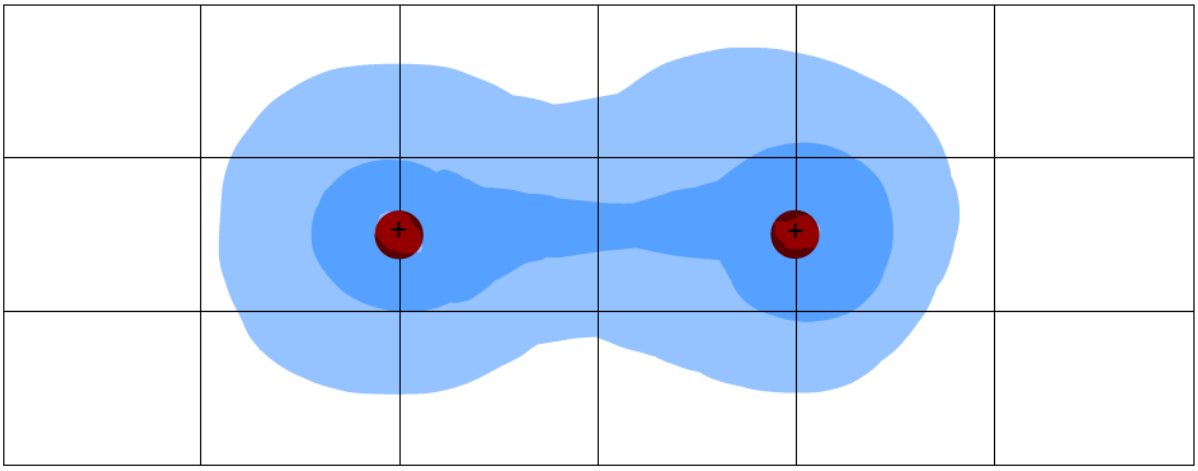
Grund für die Anziehung zwischen verschiedenen Nichtmetallatomen

Die Elektronen mit negativer Ladung werden von beiden positiv geladenen Atomkernen angezogen, was die zwei Atome als Ganzes zusammenhält. Die Distanz der Atome ist jedoch nicht beliebig nahe, da ab einer gewissen Nähe die Abstossung der positiven Atomkerne überwiegt und die Atommittelpunkte deshalb auf einer bestimmten Distanz zueinander hält. Diese Distanz wird auch als die *Bindungslänge* bezeichnet.



Darstellung der Anziehungskräfte (grün) zwischen den Bindungselektronen und den Atomkernen sowie den Abstossungskräften (rot) in einem H_2-Molekül.

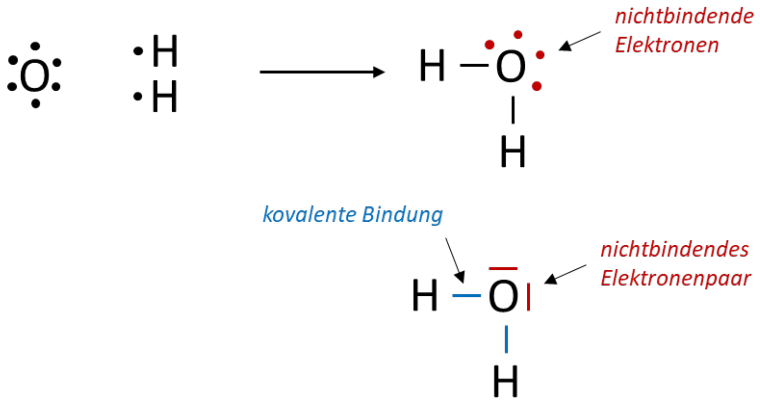
Die Aufenthaltswahrscheinlichkeit der involvierten Elektronen verschiebt sich, wenn eine kovalente Bindung zwischen zwei Nichtmetallatomen möglich ist. Bei einer Einfachbindung sind jeweils zwei Elektronen involviert, weshalb der Begriff der *Elektronenpaarbindung* oft anzutreffen ist. Dabei entsteht ein Raum zwischen den Atomkernen, in welchem die Elektronen neu anzutreffen sind. Diese gemeinsam, doppelt besetzte Elektronenwolke wird als eine kovalente Bindung bezeichnet.



Aufenthaltswahrscheinlichkeitsverteilung der zwei involvierten Bindungselektronen einer kovalenten Bindung bei einem H_2-Molekül.

Lewis-Schreibweise und das Herleiten von Lewis-Strukturformeln

Valenzelektronen werden mit Punkten dargestellt. Doppeltbesetzte Elektronenwolken als Striche. Diese werden verwendet, wenn nichtbindende Elektronenpaare auftreten oder kovalente Bindungen zwischen verschiedenen Atomen anzutreffen sind.



Valenzelektronen, kovalente Bindungen und nichtbindende Elektronenpaare in der Lewis-Schreibweise

Die maximale Anzahl an doppelt besetzten Elektronenwolken um ein Zentralatom der ersten zwei Perioden ist vier. Dies bedeutet, dass z.B. Sauerstoff in einem Wassermolekül nicht sechs kovalente Bindungen eingeht, sondern nur zwei doppelt besetzte Elektronenwolken mit Wasserstoffatomen bildet. Zusammen mit den zwei nichtbindenden Elektronenpaare sind vier doppelt besetzte Elektronenwolken um das Sauerstoffatom angeordnet.

Neben den einfachen kovalenten Bindungen sind auch zweifach- und dreifach-Bindungen möglich (siehe z.B. O_2 und N_2-Molekül).

Molekülbegriff

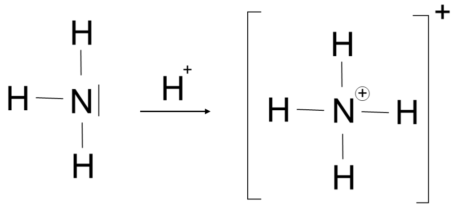
Ein *Molekül* ist ein Atomverband aus mindestens zwei nichtmetallischen Atomen, die über kovalente Bindungen miteinander verknüpft sind.

Informationsgehalt chemischer Formeln

Bei Salzen und Metallen kann lediglich das Verhältnis der Atome der enthaltenen Elemente hergeleitet werden. Beispielsweise bedeutet dies für Magnesiumiodid (MgI_2), dass doppelt so viele Iodid-Anionen wie Magnesium-Kationen enthalten sind. Bei molekularen Stoffen wird oft die Molekülformel angegeben, die sich äusserlich nicht von den Verhältnisformeln der Metalle und Salze unterscheidet. Bei molekularen Stoffen, die ausschliesslich nichtmetallische Elemente in der chemischen Formel enthalten, lassen sich direkt Schlüsse zum Aufbau der Moleküle ziehen. Die Molekülformel H_2O von Wasser gibt uns folglich die Zusatzinformation, dass ein Wassermolekül aus einem Sauerstoff- und zwei Wasserstoffatomen besteht.

Mehratomige Ionen oder Molekül-Ionen

Durch die Aufnahme bzw. Abgabe von Protonen (H^+) können Moleküle von ihrem typischerweise neutralen Ladungszustand abweichen. Dadurch entsteht aus einem Molekül ein Molekül-Ion. Solche Molekül-Ionen können wiederum als Bausteine für ionische Verbindungen verwendet werden.



Ein elektrisch neutrales Ammoniak-Molekül (NH_3) wird durch die Aufnahme eines Protons zu einem Ammonium-Ion (NH_4)$^+$.

Bei der Überprüfung der in einer Summenformel enthaltenen Elemente soll besonders auf das Ammonium-Ion geachtet werden, weil damit ionische Verbindungen mit ausschliesslich Nichtmetallen möglich sind (z.B. NH_4Cl). Salze, die Molekül-Anionen enthalten, lassen sich hingegen leichter identifizieren, da diese typischerweise in Kombination mit einem Metall-Kation auftreten (z.B. $CaCO_3$).

Räumliche Anordnung von Elektronenwolken

Die Anordnung von doppelt besetzten Elektronenwolken kann mittels des Elektronenpaar-Abstossungsmodells (EPA) hergeleitet werden (siehe Abschnitt 4.9).

Arbeitsblatt V/1: Siedetemperaturen verschiedener Stoffe

Auftrag 1: Gegeben sind die folgenden Stoffe:

MgO, H_2O, $NaCl$, CH_4, Cl_2, Al, N_2, Na, O_2, H_2

a) Versuchen Sie diese Stoffe gemäss ihrer Siedetemperatur aufsteigend einzuordnen und begründen Sie jeweils ihre Wahl. Überlegen Sie sich eine Strategie, wie Sie vorgehen könnten.

Hinweis: Überlegen Sie sich, wie die Stoffe jeweils vorliegen. Von was hängt die Siedetemperatur ab?

b) Können Sie die Stoffe den gegebenen Siedetemperaturen zuordnen?

°C Sdt	-253	-196	-183	-162	-34	+100	+882	+1465	+2470	+3600
Stoff										

c) Bei welchen Stoffen fällt ihnen eine Zuordnung besonders schwer?

Fazit:

V. Zwischenmolekulare Kräfte (ZMK)

5.1 Einstiegsexperiment

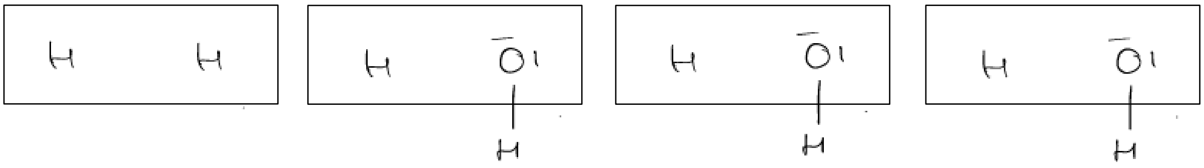
Arbeitsblatt V/2: ZMK bei Wasser

Auftrag 1: Zeichnen Sie H_2O in der Lewis-Schreibweise unter Berücksichtigung der korrekten räumlichen Anordnung.

Auftrag 2: Zeichnen Sie die zu erwartende doppelt besetzte Elektronenwolke ein:

EN: H = 2.2

EN: O = 3.5



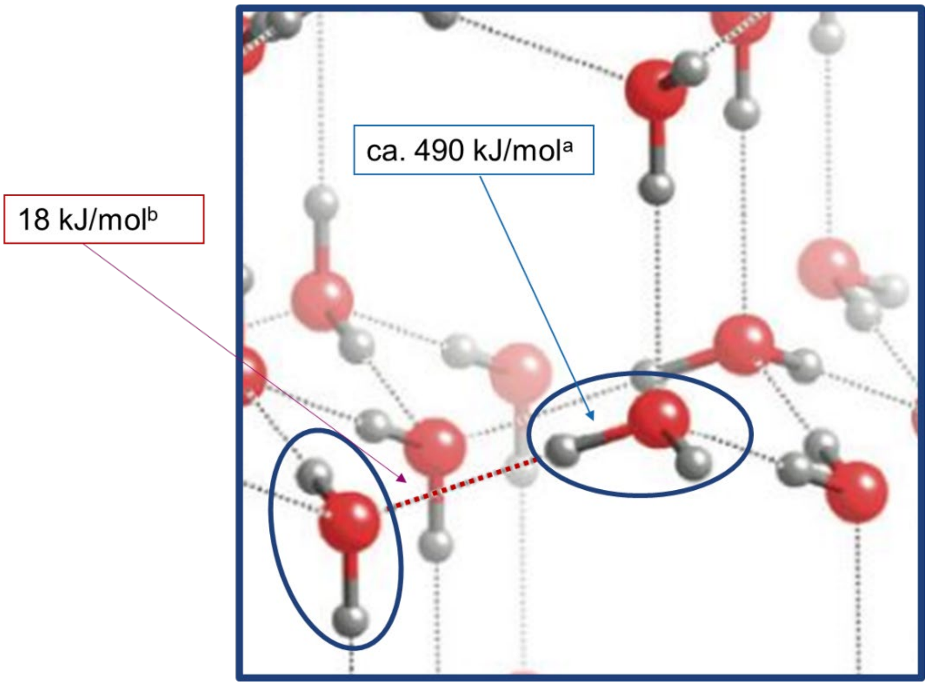
Auftrag 3: Wie werden sich mehrere Wassermoleküle anordnen?

5.2 Abgrenzung der ZMK gegenüber den kovalenten Bindungen

Die **Bindungskräfte** in einem Molekül haben Einfluss auf die Stabilität des Moleküls und somit auf die chemische Reaktivität des jeweiligen Stoffes.

Die **Zwischenmolekularen Kräfte** beeinflussen Eigenschaften wie den Schmelz- oder Siedepunkt eines Stoffes oder seine Mischbarkeit mit anderen Stoffen. Sie dürfen keinesfalls mit den Bindungskräften zwischen den einzelnen Atomen innerhalb eines Moleküls verwechselt werden.

Moleküle halten untereinander mit **zwischenmolekularen Kräften**, abgekürzt **ZMK,** zusammen. Im Innern halten Moleküle mit **kovalenten Bindungen** zusammen.

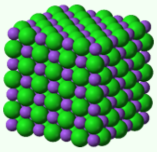
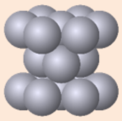
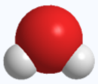


[a] *Lehninger, Albert L.; Nelson, David L.; Cox, Michael M. (2005). Lehninger Principles of Biochemistry (4th ed.). W. H. Freeman. p. 48. ISBN 978-0-7167-4339-2.*
[b] Markovitch, O.; Agmon, N., Structure and Energetics of the Hydronium Hydration Shells. *The Journal of Physical Chemistry A* **2007,** *111* (12), 2253-2256.
Bildquelle: (Nick Greeves, zugeschnitten, blaue Kreise, gepunktete Linie und Energieangaben hinzugefügt)

Auftrag 4: Können Sie erklären, wieso Wasser bereits bei 100 °C gasförmig wird, aber dabei in seinen Molekülen zusammenbleibt?

5.3 Abgrenzung der ZMK gegenüber Metallen und Ionenverbindungen

Metalle halten nur mit der **Metallbindung** zusammen, Ionenverbindungen nur mit der **Ionenbindung**. In Salzen und in Metallen gibt es keine zwischenmolekularen Kräfte.

Bindungsart	**ionische Bindung**	**metallische Bindung**	**kovalente Bindung**		
Art der Elemente	**Metalle und Nichtmetalle**	**Metalle unter sich**	**Nichtmetalle unter sich**		
Anziehung zwischen	**Anionen und Kationen**	**Atomrümpfen + Elektronengas**	**Atomrümpfen + Elektronen**		
Art der Teilchen oder Verbände	**riesiger Ionenverband,** Anordnung gemäss **Ionengitter**	**riesiger Atomverband,** Anordnung gemäss **Metallgitter**	**kleine Moleküle**		
Stoffklasse					
Abbildungen					

5.4 Relative Stärke der ZMK im Vergleich zu chemischen Bindungen

5.5 Wichtige Folge der zwischenmolekularen Kräfte

Je stärker die zwischenmolekularen Kräfte bei einem aus Molekülen bestehenden Stoff, desto höher die Siedetemperatur (Sdt). Diese Aussage gilt in ähnlicher Weise auch für die Schmelztemperatur (Smt).

5.6 Dipol-Dipol-Anziehung – der Grund für die ZMK

Wenn ein Molekül ein Dipol ist, besitzt es als Ganzes ein positives und ein negatives Ende. Nur in Ausnahmefällen ist dabei der zugehörige Dipol-Vektor kollinear mit einer Kovalenzbindung. Nähert man nun zwei Dipole einander an, so werden sie sich so ausrichten, dass der positive Pol des einen Moleküls möglichst nahe an den negativen Pol des anderen Moleküls zu liegen kommt. Dann kommt es gemäss Coulomb-Gesetz zu einer Anziehung zwischen den beiden Partialladungen der unterschiedlich geladenen Pole.

Um die Pole wieder voneinander zu trennen, muss man diese Energie entgegen der Coulomb-Anziehung aufwenden. Reicht die Energie der Umgebung nicht aus, um diese Coulomb-Anziehungskraft zu überwinden, so bleiben die Dipol-Moleküle beieinander. Auf eine grössere Menge solcher Moleküle übertragen bedeutet dies, dass der entsprechende Stoff im flüssigen oder gar im festen Zustand vorliegt. Um molekulare Stoffe in die Gasphase zu übertragen, muss dem System folglich mehr Energie, meist in Form von Wärme, übertragen werden.

Beispiel: HCl

Arbeitsblatt V/3: Dipol-Dipol-Kräfte

Auftrag 1: Die Siedetemperatur eines Stoffes hängt eng mit den Zwischenmolekularen Kräften zwischen den Molekülen zusammen. In der folgenden Lernaufgabe werden Sie erklären, wieso Methan (CH_4) mit -164°C einen sehr tiefen Siedepunkt aufweist, während Dichlormethan (CH_2Cl_2, +41°C) und Chloroform ($CHCl_3$, +61.2°C) bei viel höheren Temperaturen sieden.

a) Zeichnen Sie die drei Moleküle in der Lewisformel-Schreibweise und bestimmen Sie, ob die Moleküle einen Dipol aufweisen, indem Sie allfällige Partialladungen ($\delta+$ / $\delta-$) einzeichnen.

Methan (CH_4)

Dichlormethan (CH_2Cl_2)

Chloroform ($CHCl_3$)

b) Zeichnen Sie für die Moleküle mit Dipol je zwei Moleküle mit der zu erwartenden gegenseitigen Ausrichtung.

b) Betrachten Sie nochmals die Siedepunkte der Stoffe: Von was hängt der Siedepunkt eines molekularen Stoffes mit Dipolen ab?

Auftrag 2: CO_2 hat eine Siedetemperatur von -78 °C während HCN eine Siedetemperatur von 25 °C hat. Können Sie dies erklären?

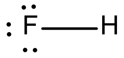
5.7 Wasserstoffbrücken – besonders starke Dipol-Dipol-Kräfte

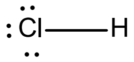
Die Besonderheit stark polarer Bindungen, an denen H-Atome beteiligt sind, beruht darauf, dass H-Atome nur ein Valenzelektron besitzen. Wenn das Wasserstoffatom über eine kovalente Bindung an ein stark elektronegatives Atom gebunden ist, dann werden die Elektronen stärker vom Wasserstoff weggezogen. Beim Atomkern des Wasserstoffatoms, welcher nur aus einem Proton besteht, entsteht auf diese Weise eine starke positive Partialladung. Solch ein stark positiv polarisiertes Wasserstoff-Atom kann eine elektrostatische Anziehung zu einem freien Elektronenpaar eines anderen Moleküls ausüben. Diese zwischenmolekulare Kraft wird Wasserstoffbrücke genannt.

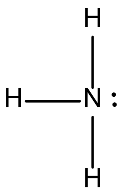
Wasserstoffbrücken sind speziell starke und gerichtete Kräfte. Diese treten nur auf, wenn bei einem Molekül ein H-Atom an ein besonders stark elektronegatives Atom (EN > 3: F, O, N) kovalent gebunden ist und am andern Molekül ein Atom mit einer stark negativen Partialladung und einem freien Elektronenpaar vorhanden ist. Das stark elektropositive H-Atom zieht ein nichtbindendes Elektronenpaar vom stark negativen Atom des andern Moleküls in seine Richtung. Der Name Wasserstoffbrücke rührt daher, dass der Wasserstoffkern sozusagen eine Brücke schlägt zwischen den stark elektronegativen Atomen beider Moleküle.

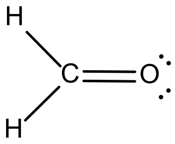
Beispiel: H_2O

Auftrag 1: Beurteilen Sie, ob die gezeichneten Moleküle Wasserstoffbrücken ausbilden können. Zeichnen Sie hierzu bei den folgenden Molekülen die Partialladungen (δ+ / δ–) ein und zeichnen Sie jeweils ein weiteres korrekt ausgerichtetes Molekül, um die Wasserstoffbrücken darzustellen.





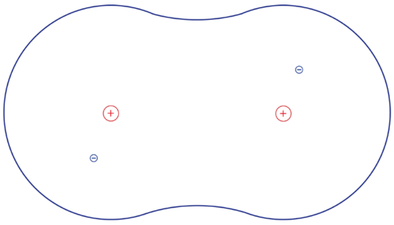




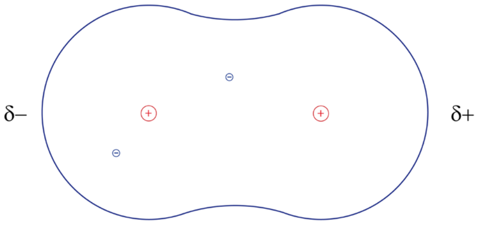
5.8 Van-der-Waals-Kräfte

Wasserstoffmoleküle (H_2) besitzen keinen permanenten Dipol, da es keine Unterschiede in der Elektronegativität gibt. Man würde deshalb vermuten, dass die Schmelztemperatur beim absoluten Nullpunkt (-273.15 °C) liegt. Messungen zeigen aber, dass die Schmelztemperatur 14 Kelvin über dem absoluten Nullpunkt liegt (-259.14 °C). Daraus folgt, dass trotz fehlendem permanentem Dipol eine Anziehung zwischen den Wasserstoffmolekülen vorhanden sein muss.

Um zu verstehen, wie diese eher schwache Anziehung zustande kommt, betrachten wir die möglichen Aufenthaltsorte der Elektronen eines Wasserstoff-Moleküls etwas genauer. Den genauen Aufenthaltsort eines Elektrons lässt sich nicht feststellen. Wenn man sich aber in einem Gedankenexperiment vorstellt, dass man Momentaufnahmen von Wasserstoffmolekülen mit ihren Elektronen macht, zeigt sich folgendes Bild:



Momentaufnahme 1: Die beiden Bindungselektronen der gemeinsamen Bindung halten sich zur Zeit der "Aufnahme" ungefähr in der Mitte auf. Die beiden negativen Ladungen sind mehr oder weniger gleichmässig verteilt, die Bindung ist unpolar und das Molekül weist keine Pole und keine Partialladungen auf.

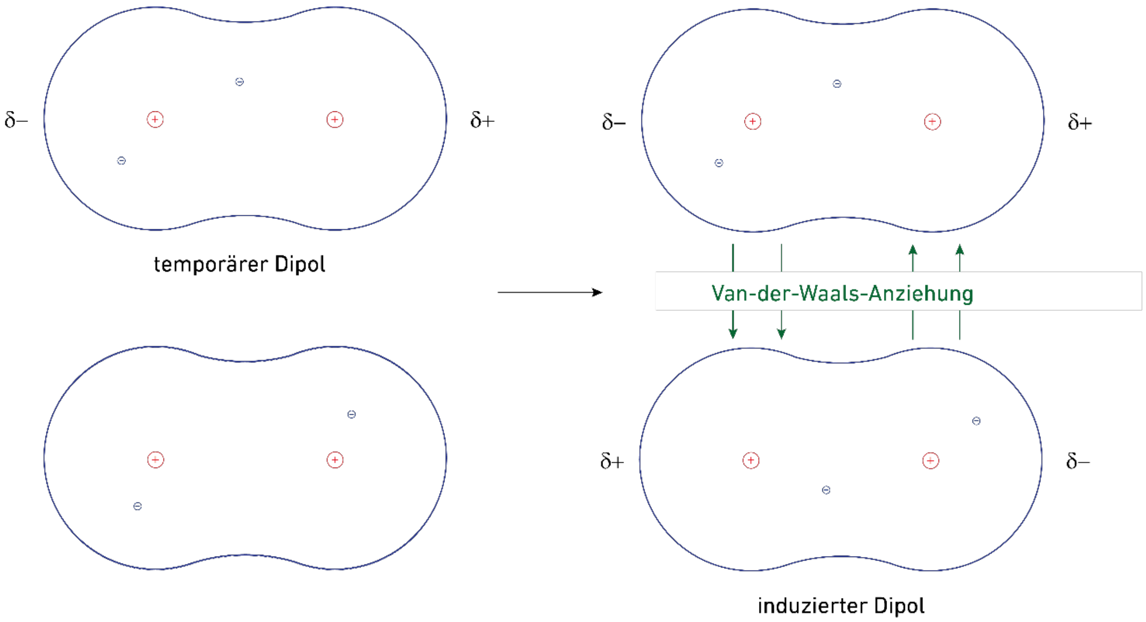


temporärer Dipol

Momentaufnahme 2: Wenn wir kurz später eine neue "Aufnahme" machen zeigt sich ein anderes Bild: Zufällig befinden sich beide Elektronen beispielsweise eher näher beim linken Wasserstoffkern. Durch diese Anordnung der beiden Elektronen bildet sich für extrem kurze Zeit ein Dipol, **ein temporärer Dipol**.

Induzierte Dipole

Wie unten illustriert, bewirkt ein temporärer Dipol, dass die Elektronenverteilung eines anderen Wasserstoff-Moleküls (links unten) ebenfalls beeinflusst wird und sich ein weiterer temporärer Dipol bildet (rechts unten). Man spricht hierbei von einem induzierten Dipol, da dieser Dipol durch ein anderes Molekül induziert worden ist. Die Vorzeichen der Partialladungen sind dabei genau entgegengesetzt.



Der temporäre Dipol, der diese Veränderung bewirkt hat, und der entstandene induzierte Dipol ziehen sich für extrem kurze Zeit gegenseitig an. Ein paar Millionstel Sekunden später sieht die Elektronenverteilung schon wieder ganz anders aus, weil sich Elektronen nicht an einem festen Ort aufhalten.

Diese temporären Dipol-Kräfte sind aber dafür verantwortlich, dass unpolare Verbindungen, wie beispielsweise Wasserstoff, Methan oder Hexan, Schmelzpunkte aufweisen, die höher als der absolute Nullpunkt liegen. Man bezeichnet die Anziehung zwischen solchen temporären und induzierten Dipolen als **Van-der-Waals-Kräfte**. Gäbe es diese Van-der-Waals-Anziehungskraft nicht, so wären Verbindungen ohne permanentem Dipol selbst bei den tiefsten Temperaturen gasförmig und nicht, wie beispielsweise Hexan, bei Zimmertemperatur flüssig. Der Elementarstoff Iod, der ebenfalls aus völlig unpolaren I_2-Molekülen besteht, ist bei Zimmertemperatur aufgrund der Van-der-Waals-Anziehungskräften zwischen den Iod-Molekülen sogar fest.

Arbeitsblatt V/4: Van-der-Waals-Kräfte und Vergleich aller ZMK

Auftrag 1: Betrachten Sie die folgende Tabelle.

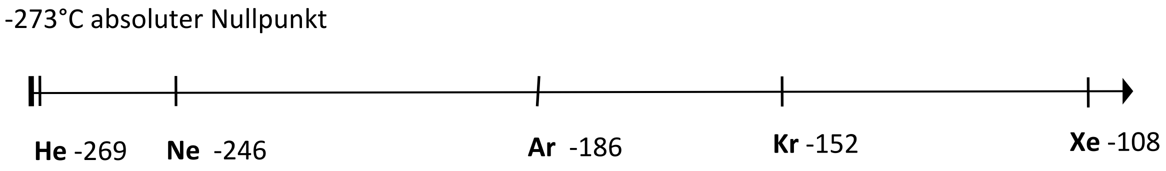
	F_2	**Cl_2**	**Br_2**	**I_2**
Schmelztemperatur in °C bei Atmosphärendruck	-220	-102	-7	114
Siedetemperatur in °C bei Atmosphärendruck	-188	-34	59	186
Aggregatzustand bei Raumtemperatur				

a) Tragen Sie den bei Raumtemperatur (25° C) vorherrschenden Aggregatzustand der verschiedenen Stoffe ein.

b) Zeichnen Sie F_2 in der Lewis-Formel und überlegen Sie sich, ob das Molekül einen Dipol aufweist oder nicht. Wie sieht es für die anderen Stoffe aus?

c) Haben Sie eine Vermutung, woran dass es liegen könnte, dass die Schmelz- und Siedetemperaturen von F_2 bis I_2 zunehmen?

Auftrag 2: Edelgase existieren als einzelne Atome. Da Sie keine Bindungen eingehen, können diese auch keine Dipole bilden. Dennoch ist der Siedepunkt der Edelgase teilweise deutlich über dem absoluten Nullpunkt (-273 °C).



a) Die Siedetemperaturen steigen systematisch an. Können Sie eine Regel herleiten?

b) Bei Edelgasen wirken ebenfalls Van-der-Waals-Anziehungskräfte. Inwiefern ist es speziell, wenn man hier von zwischenmolekularen Kräften spricht?

Auftrag 3: Was haben alle ZMK (H-Brücken, Dipol-Dipol-Wechselwirkungen und Van-der-Waals-Kräfte) gemeinsam?

Auftrag 4: Versuchen Sie die folgende Übersichtstabelle auszufüllen.

	VdW	**D-D**	**H-Brücken**
Grund für die Anziehung zwischen Molekülen			
Relative Stärke der Anziehungskraft			
Anziehungskraft desto grösser, je …			

5.9 Übersicht der zwischenmolekularen Kräfte

Bei welchen Stoffen sind zwischenmolekulare Kräfte feststellbar?

Zwischenmolekulare Kräfte treten, wie der Name andeutet, ausschliesslich *zwischen Molekülen* auf. Edelgase werden nicht als Moleküle bezeichnet, da sie als Einzelatome vorliegen. Dennoch sind bei Edelgasen zwischenmolekulare Kräfte feststellbar. Bei ionischen oder metallischen Verbindungen treten hingegen keine zwischenmolekularen Kräfte auf.

Welche Arten von zwischenmolekularen Kräfte gibt es und worin liegt der Ursprung der Anziehungskräfte?

Die zwischenmolekularen Kräfte werden in drei Arten eingeteilt:

- **Van-der-Waals-Kräfte (VdW)**
- **Dipol-Dipol-Kräfte (D-D)**
- **Wasserstoffbrücken (Wbr)**

Alle drei zwischenmolekularen Kräfte treten auf, wenn Elektronen nicht gleichmässig über das Molekül verteilt sind. Wenn sie sich bei einem Molekül an einer Stelle Elektronen konzentrieren, bildet sich dort ein negativer Pol. Weist hingegen ein Nachbarmolekül an einer Stelle zu wenig Elektronendichte auf, tritt dort ein positiver Pol auf. Die beiden Pole und damit die beiden Moleküle ziehen sich durch die Coulombkraft an, was man als zwischenmolekulare Kraft bezeichnet. Beachte dabei, dass die Anziehung um mindestens eine Grössenordnung zehn bis hundert kleiner ist als die Coulomb-Anziehung zwischen Ionen, bei welchen vollständige Ladungen auftreten.

Wie werden die zwischenmolekularen Kräfte unterschieden?

Die beiden Pole entstehen bei den drei zwischenmolekularen Kräften auf unterschiedliche Weise:

- Durch grössere Unterschiede in der Elektronegativität von verschiedenen Atomen kommt es vor, dass die Elektronendichte an gewissen Stellen im Molekül grösser ist. Dadurch weisen solche Moleküle einen **permanenten Dipol** auf. Diese Moleküle bilden **Dipol-Dipol-Kräfte** aus.
- F, O und N verfügen über eine besonders grosse Elektronegativität. Wenn diese Atome ein H gebunden haben, können sich speziell starke permanente Dipole bilden. Die ausgebildeten Anziehungskräfte zwischen den Molekülen werden als **Wasserstoffbrücken** bezeichnet.
- Besitzt ein Molekül keinen permanenten Dipol, so ist es immer noch möglich, dass eine Anziehung zwischen temporären und induzierten Dipolen auftritt. Diese Anziehungskraft wird als **Van-der-Waals-Kraft** bezeichnet.
- Die Stärke der Zwischenmolekularen Kräfte nimmt in der Reihenfolge
  Van der Waals-Kräfte → Dipol/Dipol-Wechselwirkung → Wasserstoffbrücke deutlich zu.

Es ist zu beachten, dass eine an sich stärkere zwischenmolekulare Kraft von einer an sich schwächeren übertroffen wird, wenn die schwächere Kraft mehrmals zwischen den betrachteten Molekülen wirkt.

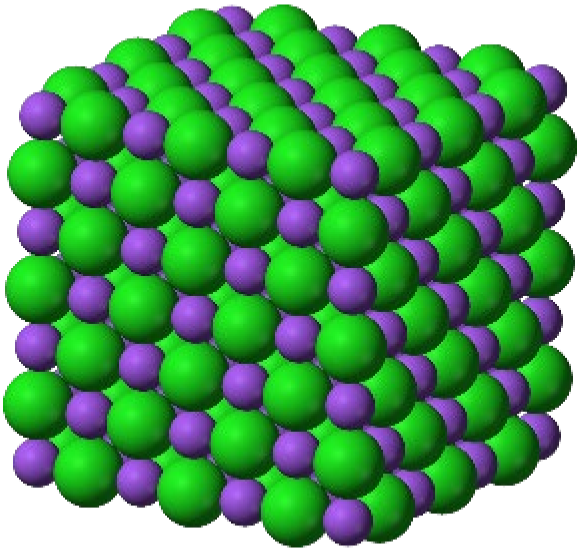
5.10 Rückbezug zur ersten Lektion zu chemischen Bindungen

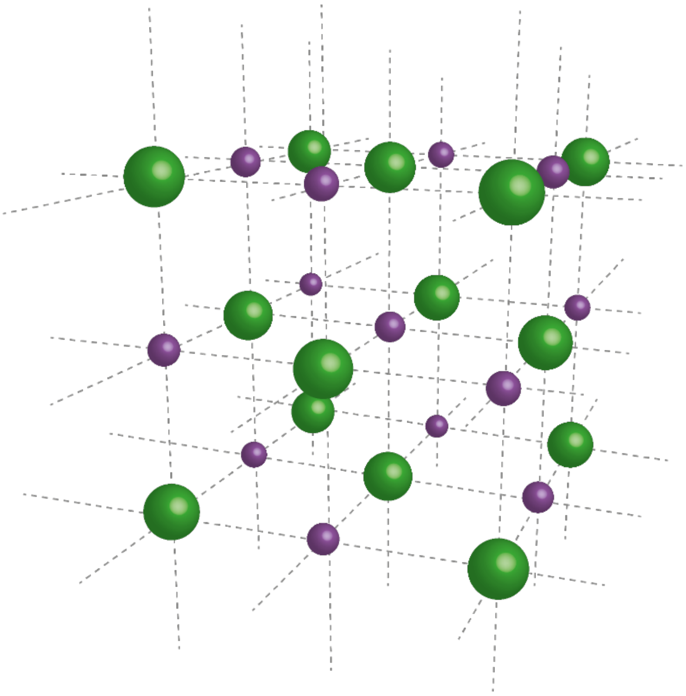
Tab. 1: Eis, Natriumchlorid und Diamant (Rob Levinsky (n.b.)) mit den Schmelztemperaturen.

Wasser	**Natriumchlorid**	**Diamant**
H_2O	NaCl	C
		
Schmelztemperatur		
0 °C	801 °C	Etwa 4 000 °C

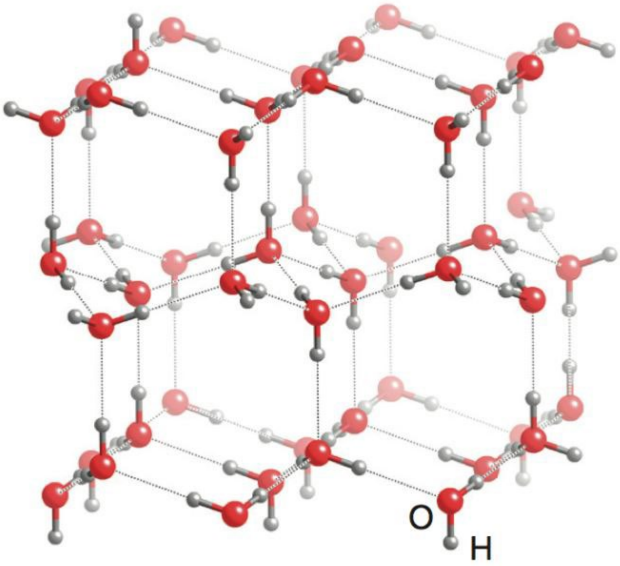
AB V/ 5: Vergleich eines Salzkristalls mit einem Eiskristall

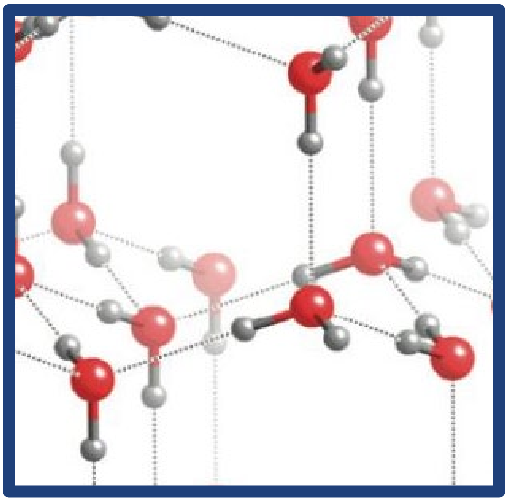
Auftrag 1: Vergleichen Sie Natriumchlorid (NaCl) in Form eines Salzkristalls mit einem Eiswürfel (H_2O)





Um etwas besser in das Innere des Salzes zu sehen, wurden die **Natriumkationen (violett)** und **Chlorid-Anionen (grün)** etwas auseinander gezeichnet.





Bildquelle: Nick Greeves, n.d. links (belassen), rechts (vergrössert und zugeschnitten)

a) Umrahmen Sie in der blau umrahmten Abbildung zwei Wassermoleküle.

b) Wie liegen die Atome vor in den beiden Verbindungen?

c) Wie halten die Teilchen in H_2O zusammen?

d) wie halten die Teilchen in NaCl zusammen?

e) Zeichnen Sie die ZMK bei den Stoffen ein. Wie werden diese ZMK genannt?

f) Wie viele Bindungspartner haben die fett markierten Atome?

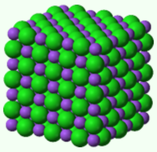
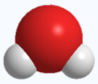
Na**Cl**

H_2**O**

g) Zeichnen Sie Wasser bei 100 °C

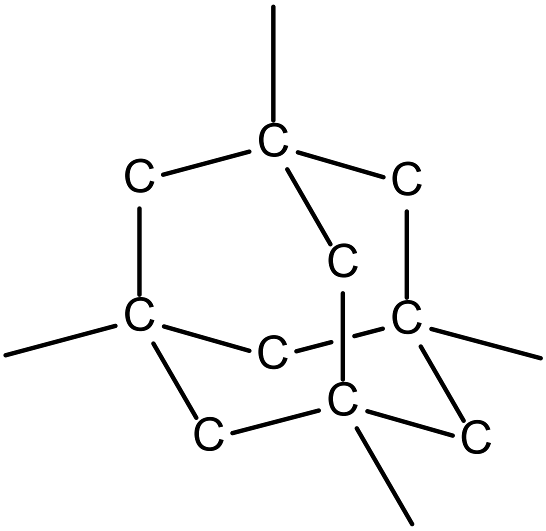
5.10.1 Dipol-Dipol-Wechselwirkung bei Molekülen und Coulombanziehung in einer ionischen Verbindung im Vergleich

5.10.2 Schmelzen und Sieden bei verschiedenen Bindungssituationen

Bindungsart	**ionische Bindung**	**metallische Bindung**	**kovalente Bindung**		
Art der Elemente	**Metalle und Nichtmetalle**	**Metalle unter sich**	**Nichtmetalle unter sich**		
Anziehung zwischen	**Anionen und Kationen**	**Atomrümpfen + Elektronengas**	**Atomrümpfen + Elektronen**		
Art der Teilchen oder Verbände	**riesiger Ionenverband,** Anordnung gemäss **Ionengitter**	**riesiger Atomverband,** Anordnung gemäss **Metallgitter**	**kleine Moleküle**		
Stoffklasse					
Abbildungen					

5.10.3 Diamantstruktur

Am Anfang dieser Unterrichtseinheit haben Sie erfahren dass der Schmelzpunkt eines Diamanten bei über 4000 °C liegt. Wenn man die Zusammensetzung anschaut, sieht man, dass kovalente Bindungen enthalten sein müssen und demnach der Stoff aus Molekülen bestehen müsste. Wie ist aber ein solch hoher Schmelzpunkt mit dem Wissen vereinbar, dass ZMK deutlich schwächer sind? Die Antwort ist bestechend einfach: In einem Diamanten kommen keine ZMK vor, da in einem Diamanten alle Atome mit kovalenten Bindungen miteinander verknüpft sind. Jedes Kohlenstoffatom kann sich mit vier weiteren verbinden. Ein Diamant besteht folglich aus einem einzelnen «Riesenmolekül». Um diese Struktur flüssig oder gasförmig werden zu lassen müssen demnach kovalente Bindungen gebrochen werden, was nur mit viel Energie möglich ist, was auch den hohen Schmelzpunkt gut erklärt.



Veranschaulichung der Verknüpfung der C-Atome in einem Diamanten.