DESIGN-BASED RESEARCH: THE USE OF COMPUTER-BASED MOLECULAR MODELLING TO ENHANCE STUDENT UNDERSTANDING OF CHEMICAL BONDING

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Tiivistelmä – Referat – Abstract

Bonding is a central concept in chemistry education; thus a thorough understanding of it is crucial in order to understand various other concepts of chemistry. However, students often find it difficult to understand the concept of bonding and as a result develop alternative conceptions. Living in a macroscopic world, students may find it difficult to shift between macroscopic and molecular levels; this is one of the reasons why students find it difficult to understand chemical bonding. The wide range of complex and sophisticated scientific models that scientists have developed to explain bonding, can be confusing for students. Moreover, students develop alternative conceptions as a result of the way they are taught. Computer-based molecular modelling could be utilized to facilitate and enhance student understanding of bonding.

This thesis describes a study on the supportive opportunities and challenges encountered when using computer-based molecular modelling to enhance student understanding of bonding, focusing particularly on three main inquiries. Investigating the challenges students face when utilizing computer-based molecular modelling to understand and explain chemical bonding. Exploring the features of computer-based molecular modelling that enhance student understanding of bonding. And analysing how to optimally support students understanding of bonding when using computer-based models.

The study was conducted as a design-based research, centred particularly on student's opinions. An exercise was designed and implemented with 20 International Baccalaureate (11^{th} grade students) during their chemistry lessons. The exercise sheet comprised of brief explanations on bonding, instructions to visualize models on Edumol (a web based molecular modelling and visualization environment) and questions to be answered after visualizing the models.

The research results highlighted the importance of well planned activities to ensure the effective use of computer-based models. Prior to using computer-based models in class, teachers must consider possible solutions for technical difficulties that might arise. They must also plan activities based on student's prior experiences with models, to ensure that nothing hinders the students learning process. Additionally, teachers must individualize activities by taking into consideration students opinions and preferences, to ensure productive learning. Furthermore, teachers should optimize the use of the effective features of computer-based models. Features such as molecular electrostatic potentials, that are only possible to visualize via computer-based models. Finally, teachers should use the necessary supportive materials in conjunction with the computer-based models to enhance student understanding of bonding.

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Dedicated to my mother

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1. Introduction

According to previous researches (Feller et al., 2004; Hessley, 2004; Tasker and Dalton, 2006; Barak & Dori, 2005) computer-based molecular modelling enhances student understanding of chemistry and chemical bonding. Nevertheless, few researches have been conducted to analyse how to support the use of computer-based molecular modelling in the classroom to ensure that students have a productive experience. The aim of this research is to evaluate how to support the use of computer-based molecular modelling to enhance student understanding of bonding. The study mainly aims to evaluate the possible challenges that teachers and students encounter, to recognize the features of computer-based molecular modelling that promotes and enhances student understanding of bonding, and to perceive how to optimally support students learning experiences.

Chemical bonding is one of the basic fundamental concepts in chemistry. Many of the concepts taught in high school and university level chemistry courses, are highly dependent on the understanding of chemical bonding. Nevertheless, according to research (Taber & Coll, 2002; Levy, Nahum, Mamlok-Naaman, Hofstein & Taber, 2010; Gabel, 1996; Harrison & Treagust, 2000, Johnstone, 1991; Robinson, 2003) the concept of bonding is one of the most difficult concepts for students to comprehend. This is because living in a macroscopic world, students find it difficult to shift between macroscopic and molecular levels (Gabel, 1996; Harrison & Treagust, 2000, Johnstone, 1991; Robinson, 2003); thus, they develop alternative conceptions. Moreover, according to Taber & Coll (2002), most alternative conceptions in chemistry do not result from the learner's experiences of the world but from prior science teaching. In other words, most often student's alternative conceptions are a result of how they have been taught.

Throughout the years, many researches have been conducted highlighting ideas on how the concept of bonding should be taught in order to prevent students from developing alternative conceptions. This research utilizes these many findings as well as computer-based molecular modelling to design an activity/exercise, to enhance student understanding of chemical bonding. The study aims to examine the research questions that follow. What challenges do students face when using computer-based molecular modelling software to understand and explain chemical bonding? What features of computer-based molecular modelling support students in acquiring a deeper understanding of chemical bonding? How to optimally support student understanding of chemical bonding when using computer based molecular modelling?

The research conducted is a design-based research for which an activity/exercise was designed. The exercise required students to visualize models on Edumol (a web based molecular modelling and visualization environment) and answer questions which require students to explain various chemical phenomena (see appendices 1 and 3). The aim of the exercise was to enhance student understanding of chemical bonding by facilitating three dimensional visualizations. A description of the questions in the exercise, and the rationale for each question posed is presented in detail in chapter 5.1

This thesis consists of 7 chapters. Chapter 2 is an introduction to design-based research in education, including a description of the theoretical problem analysis and design procedure for this thesis. Chapter 3 presents the theory of chemical bonding in high school chemistry, including the theory of chemical bonding and information from previous researches on how to teach chemical bonding. Chapter 4 discusses computer-based molecular modelling. Chapter 5 presents the design product, including details regarding the design of the modelling exercise, implementation in a classroom and the design of the questionnaire. Chapter 6 introduces the data analysis and results, including a description of the data analysis method, a presentation of the results, an evaluation of the reliability of the results and a contemplation of possible improvements to the design. Finally, chapter 7 presents the conclusions and discussion.

2. Design-based Research in Education

Design-based Research (Brown, 1992) is "the systematic study of designing, developing and evaluating educational interventions (such as programs, teaching-learning strategies and materials, products and systems) as solutions for complex problems in educational practice, which also aim at advancing our knowledge about the characteristics of these interventions and the processes of designing and developing them" (Nieven et al., 2012, p.13). Design research utilizes the design process in order to promote the researchers understanding of teaching, learning and educational systems (Edelson, 2002).

Design research is an ideal research method for educational research, as it aims to develop solutions for complex educational problems in educational practice based on research. The research process in design research involves a cyclic process. A problem is identified, after which, a solution to the problem is developed, the solution is then tested, evaluated and refined. Then the entire process is repeated until a balance is achieved. Reeves (2006), portrays design-based research as seen in figure 1 below. (Nieven et al., 2012)

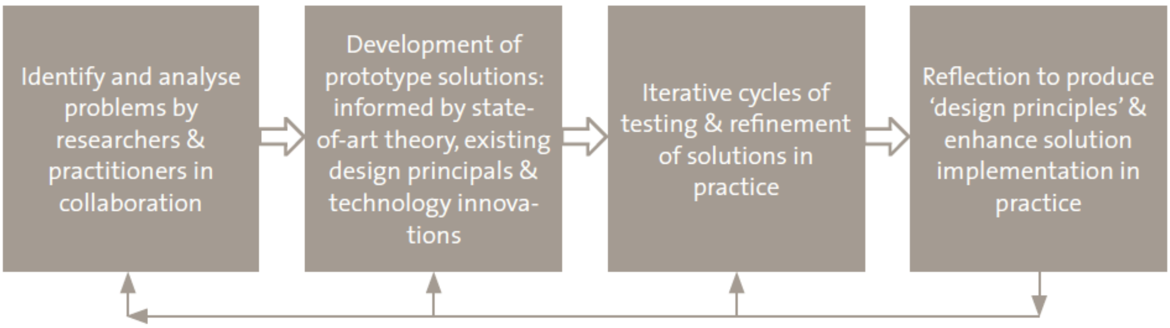


Figure 1: Cyclical Design-based Research Process (Reeves, 2006)

Any design process can be characterized by three collections of decisions that determine a design outcome: the design process, the problem analysis, and the design solution. The design process establishes the details of the process and the designers involved in developing a design. Design can prove to be a complex process, requiring a wide range of expertise and well planned systematic processes in order to ensure that the goals are met. The problem analysis highlights the goals, needs, or opportunities that the design intends to address. A design process often begins with a problem or opportunity and an idea for how to respond to it. The design product describes the developed design. It is the product of the designer's efforts to address the problems and challenges that were realized in the problem analysis. The product construction decomposes a complex design problem into manageable components. The product construction is a process of generating alternative solutions and analysing their productivity. (Edelson, 2002)

2.1 Design Research in this Thesis

This chapter first presents the theoretical problem analysis for the research, after which, the specific research questions addressed throughout the research are reported. Then finally, a detailed description of the design process is presented.

2.1.1 Theoretical Problem Analysis

Research (Taber & Coll, 2002; Levy, Nahum, Mamlok-Naaman, Hofstein & Taber, 2010; Gabel, 1996; Harrison & Treagust, 2000, Johnstone, 1991; Robinson, 2003) has confirmed that bonding is one of the most difficult concepts for students to grasp. Understandably so, as chemists use various complex and sophisticated scientific models to explain chemical bonding. Students often find it difficult to visualize these scientific models three dimensionally and hence fail to understand bonding concepts without developing alternative conceptions. Additionally, living in a macroscopic world, students often find it difficult to make productive connections between macroscopic and sub-microscopic levels; thus, hindering their understanding of the effects of bonding. Furthermore, students develop alternative conceptions as a result of way they are taught the concept of bonding. Further details regarding the difficulties students face in understanding the concept of bonding is highlighted in chapter 3.2. (Taber & Coll, 2002; Levy, Nahum, Mamlok-Naaman, Hofstein & Taber, 2010)

A possible solution for the problems that students face, is the use of computer-based molecular modelling. Molecular models, both real or computer based are highly efficient tools to facilitate visualizations (Aksela & Lundell, 2008). Additionally, according to Barak and Dori (2005), using computer-based models helped promote students' understanding of chemistry at four levels: the macroscopic, microscopic, symbolic and chemical process levels. However, using computer-based models effectively is not always straight forward and few researches have been conducted to study how to support the use of computer-based modelling in order to ensure a productive experience for students. Hence, this study researches how to support using computer-based molecular modelling to enhance student understanding of chemical bonding.

A modelling exercise was designed taking into consideration the numerous difficulties students face when learning about bonding. The aim of the research was to evaluate how to support students use of computer-based molecular modelling to enhance student understanding of bonding. The specific research questions are highlighted in chapter 2.2.2 below.

2.2.2 Research Questions

The research was conducted in order to acquire an understanding of how to optimally use computer-based molecular modelling in a class room environment in order to enhance student understanding of bonding. This was achieved by researching the challenges students face when using computer-based molecular models, researching how to optimally support students use of molecular modelling software, and researching the features of computer-based molecular modelling that enhances student understanding of chemical bonding. The research questions were specifically as follows:

1. What challenges do students face when using computer-based molecular modelling software to understand and explain chemical bonding?

2. What features of computer-based molecular modelling support students in acquiring a deeper understanding of chemical bonding?

3. How to optimally support student understanding of chemical bonding when using computer-based molecular modelling

2.2.3 Design Process

An exercise on bonding was developed (see appendix 1), in which students utilize Edumol (a web based molecular modelling and visualization environment) in order to answer questions posed. The aim of the exercise was to enhance students understanding of chemical bonding by facilitating three dimensional visualizations.

The process of developing the exercise involved taking into consideration the findings of various previous researches conducted regarding teaching chemical bonding (See chapter 3.2). The main idea was to study the suggestions that previous researches provided and to discover the common alternative conceptions that students develop when learning about bonding. The exercise was then developed based on previous studies in order to inhibit student's alternative conceptions and promote a deep understanding of bonding. The exercise was designed for students to visualize molecules and their properties on Edumol and answer questions posed. The questions aimed to ensure that students focus on the details that previous studies consider significant in order to understand bonding.

A questionnaire (Appendix 2) was then developed in order to acquire an insight into student's opinions on the exercise and their understanding. Further details regarding the design of the questionnaire can be found in chapter 5.3.

The exercise was then implemented with 20 International Baccalaureate students (11^{th} graders), in order to gauge the effectiveness of the exercise as well as to obtain insight into the earlier mentioned research questions. Prior to the implementation of the exercise the students were first briefed on what a concept map is, after which, they were required to create concept maps on chemical bonding before they studied the topic with their teacher. This was done in order to allow students to reflect on what they know and what they don't know about bonding prior to studying the topic. After studying the topic with their teacher they were then required to edit their earlier concept maps on chemical bonding, in order to reflect on their knowledge of bonding at this point. The students were then finally given the designed modelling exercise to complete, after which they were required to edit their concept maps further; hence, reflecting on their knowledge at this point as well. The students were also requested to fill in a questionnaire (appendix 2), encouraging them to express their opinions about their experience.

The evaluation of the earlier mentioned research questions and the effectivity of the modelling exercise was carried out by analysis of data acquired mainly from the questionnaire (appendix 2). Some data was also acquired from the concept maps and observations during the research process. The responses from the questionnaires and observations from the entire process provided much insight into the challenges students face when using computer-based molecular modelling, useful features of computer-based molecular modelling for understanding bonding and the possible factors that could support the use of computer-based molecular modelling.

Further details regarding the initial design product are presented in chapter 5.1. Chapter 5.2 presents the initial suggestions for the implementation in a classroom environment. Based on the research, the initial design for the exercise as well as the initial suggestions for the implementation in a classroom environment were revised and are presented in chapter 6.4.

Resources used for the Research

Edumol

Edumol is an open molecular modelling and visualization environment, which is designed specifically for chemistry teachers and students needs. It is touch compatible with all browsers except for Internet Explorer.

Cmap Cloud

The concept maps were created and edited on Cmap Cloud, in order to make it easier for students to edit their concept maps. Cmap cloud is a web-based version of CmapTools which allows users to construct, save, edit and share concept maps (Institute for Human and Machine Cognition, 2015).

3. Chemical Bonding in High School Chemistry

According to the Finnish National Curriculum chemical bonding is taught in High school during the second course of chemistry "The Micro world of Chemistry (KE2)" and according to the International Baccalaureate (IB) curriculum Chemical Bonding is covered in topic 4 "Chemical Bonding and Structure" (Finnish National Board of Education, 2003; International Baccalaureate Organization, 2016). The first section of the chapter is a description of the theory of chemical bonding that is covered in high school chemistry, reflecting both mentioned curricula. The second section of this chapter is regarding teaching chemical bonding, it reports the findings of various researches conducted about teaching chemical bonding.

3.1 Theory of Chemical bonding

This chapter specifically goes through the theory of Ionic, Covalent and metallic bonding focusing particularly on intramolecular bonding, intermolecular forces, and the physical properties of substances. Additionally, the similarities and differences between various types of bonding are discussed as well. Then finally, the theory of relative bond length is presented. Figure 2 below presents an overview of the types of bonding that have been presented in this chapter.

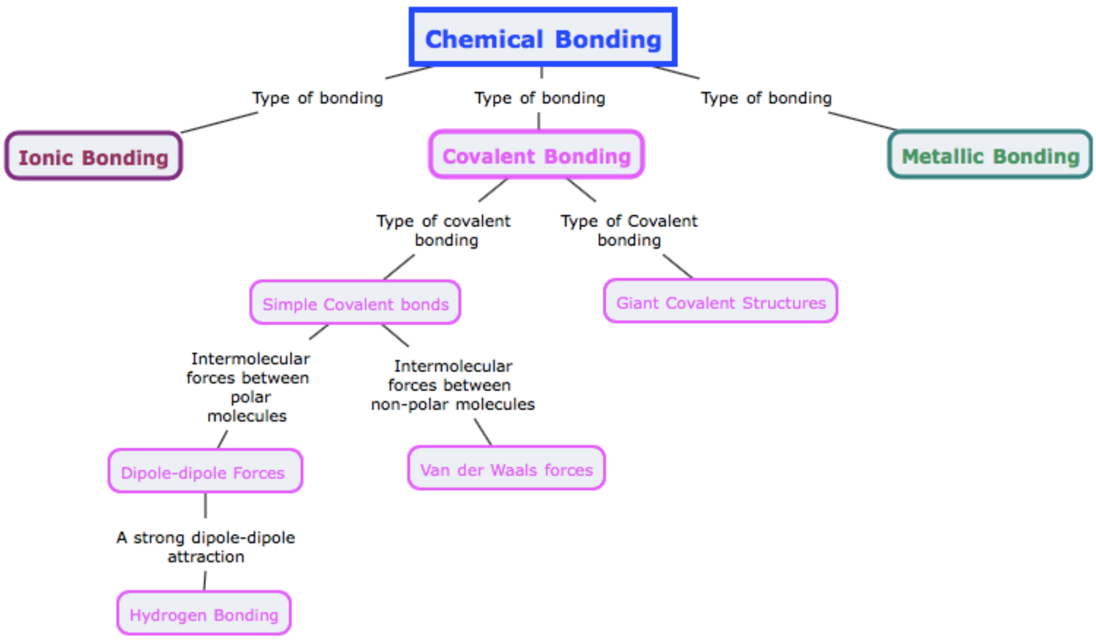


Figure 2: An overview of the types of bonding being presented in chapter 3.1

3.1.1 Ionic Bonding

Metals have a tendency to lose electrons and non-metals have a tendency to gain electrons, in order to achieve an inert gas configuration. When electrons are transferred from a metal to a non-metal in order to form ions with inert gas configurations, the metal atom forms a cation and the non-metal atom forms an anion. These oppositely charged ions are then attracted to each other by strong electrostatic forces, forming ionic bonds, that build up into strong lattice structures. A classic example of an ionic compound is sodium chloride Na^+Cl^- (table salt). An atom of sodium loses an electron and transfers it to an atom of chlorine which gains an electron. Thus creating a pair of oppositely charged ions that are attracted to each other and held together as part of a crystalline lattice. Figure 3 below depicts the formation of sodium chloride as illustrated in textbooks. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

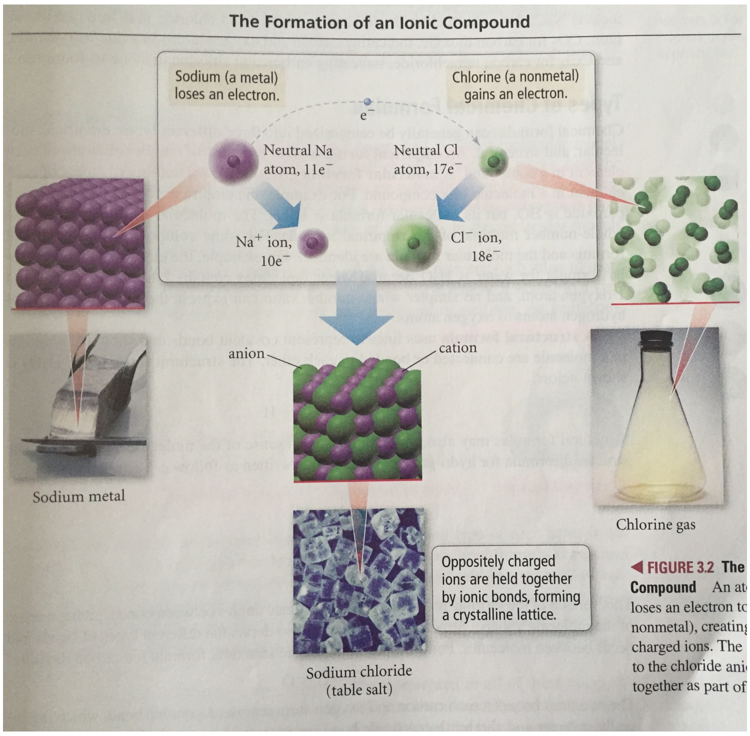


Figure 3: The formation of sodium chloride, an ionic compound (Nivaldo, 2011)

Ionic compounds have distinct properties; they conduct electricity when dissolved in water or when molten. They are soluble in polar solvents. They are relatively hard and brittle. And they have high melting points and low volatility. Ionic compounds conduct electricity when in aqueous solutions because, in aqueous solutions the ions dissociate and are free to move around and thus carry a charge through the solution. Similarly, when ionic crystals are melted, the ions are free to move around and thus conduct electricity. Ionic crystals dissolve in polar solvents since polar substances have partially positive and partially negative ends. These partially charged parts of the molecules of polar solvents attract the charged ions in ionic compounds; thus dissociating the ionic molecules. Ionic crystals are relatively hard due to the strong electrostatic attractions between oppositely charged ions in the crystals, and brittle due to the repulsion of like charged ions if they come into contact with each other. Hitting the crystal with an object could quite easily shift the arrangement of the lattice causing like charges to repel and break off. Finally, due to the strong electrostatic attraction between oppositely charge ions, ionic crystals also tend to have high melting and boiling points and low volatility. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

3.1.2 Covalent bonding

There are mainly two types of covalently bonded compounds, simple covalent compounds and giant covalent compounds. Simple covalent compounds posses two different types of intermolecular forces depending on the nature of the compound in question. Polar compounds have dipole-dipole intermolecular forces and non-polar compounds have Van der Waals intermolecular forces.

Simple Covalent Compounds

As stated earlier non-metals have a tendency to gain electrons in order to achieve an inert gas configuration. Covalent bonding occurs when non-metals bond together by sharing their outer shell electrons in order to achieve an inert gas configuration. Hydrogen (H_2) is the simplest example of a covalent compound. Hydrogen atoms consist of one electron each in their outer shells. Two covalently bonded hydrogen atoms share each of their outer shell electrons; hence both electrons (one from each hydrogen) are attracted electrostatically by both positive nuclei. Chlorine atoms bond covalently to form a chlorine molecule as depicted in figure 4 below. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

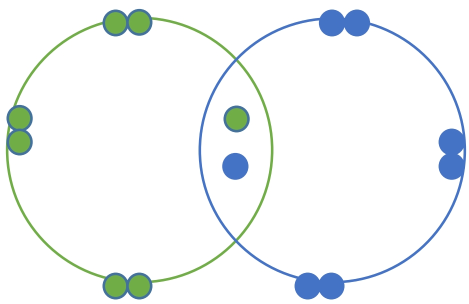


Figure 4: A chlorine molecule covalently bonded

Covalent bonds between atoms **within** a molecule are very strong; however, the forces of attraction **between** the molecules are generally much weaker. These intermolecular forces depend on the polarity of molecules. Polar molecules are held together mostly by **dipole-dipole** intermolecular forces between molecules and non-polar molecules are held together mostly by **Van der Waals forces** between molecules. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011; Kirouac & Consiglio)

Dipole-dipole forces

Covalent bonds in which electrons are shared relatively equally result in non-polar molecules such as Cl_2 and covalent bonds in which electrons are shared unequally result in polar molecules such as HCl. Electrons are generally shared equally between two atoms with the same electronegativity. When atoms bonding together have different electronegativity's, such as HCl, then the electrons are displaced toward the more electronegative atom. This results in a polar molecule with a partial positive charge at one end and a partial negative charge at the other end. Hence polar molecules are attracted to each other by electrostatic forces called dipole-dipole forces. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011; Kirouac & Consiglio)

Hydrogen bonds

Hydrogen bonding is a strong dipole-dipole attraction. It occurs when hydrogen is bonded directly to small, highly electronegative atoms such as fluorine, oxygen or nitrogen. As the electron pair is drawn away from the hydrogen atom by the electronegative atom, all that remains is the proton in the nucleus since there are no inner electrons. The proton then attracts a non-bonding pair of electrons from the F, O or N. There are three main reasons why hydrogen bonds are so strong. Firstly, because of the high difference in polarity of F-H, O-H, and N-H. Secondly, because the small sizes of the atoms ensure that the charges are highly concentrated. And thirdly, due to the small sizes of the atoms involved, the positive end of one dipole can get quite close to the negative end of another. Figure 5 below portrays a visualization of hydrogen bonding in water as illustrated in textbooks. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011; Kirouac & Consiglio)

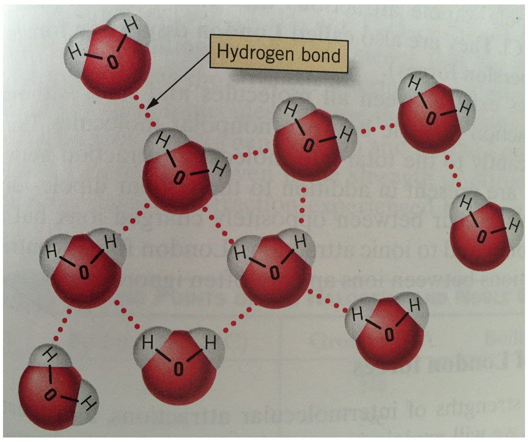


Figure 5: Hydrogen bonding in water (Brady & Senese, 2004)

Van der Waals' forces

Even in non-polar covalent molecules (such as He) the electrons can be unevenly spread at any moment, producing temporary instantaneous dipoles. An instantaneous dipole can induce another dipole in neighbouring particles resulting in weak attractions between two particles, as illustrated in figure 6 below by Kirouac & Consiglio. Van der Waals forces increase with increasing mass since a large electron cloud is more easily deformed than a small one. Because large molecules have stronger charges on oppositely charged ends of an instantaneous dipole. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011; Kirouac & Consiglio)

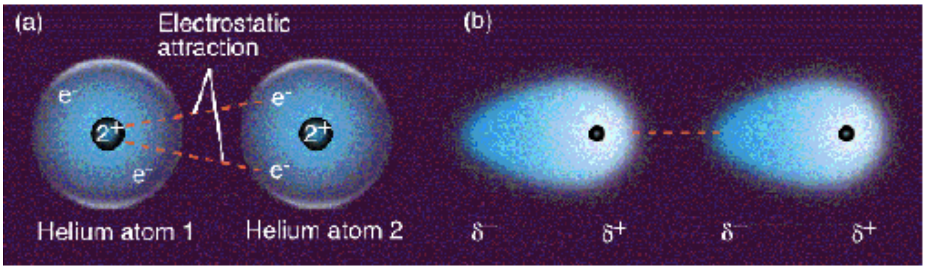


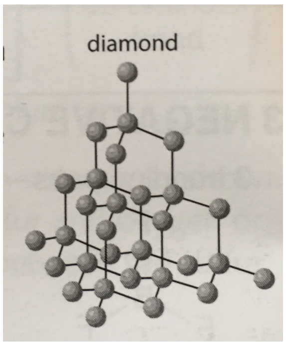
Figure 6: Induced dipole of a helium atom (Kirouac & Consiglio)

Physical properties of substances are mostly a result of intermolecular interactions. Simple covalent compounds have distinct properties, they have low melting and boiling points, and high volatility. They do not conduct electricity in solutions. And they are soluble in non-polar solvents. The low melting and boiling points, and high volatility of simple covalent compounds is due to the weak intermolecular forces between molecules. Because the forces that need to be overcome in order to melt, boil or evaporate are relatively weak. Simple covalent compounds do not conduct electricity even when aqueous because they do not transfer electrons unless they undergo a chemical reaction. Finally, covalent compounds are soluble in non-polar solvents since 'like dissolves like'. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011; Kirouac & Consiglio)

Giant Covalent Structures

Giant Covalent structures contain numerous atoms joined to adjacent atoms by covalent bonds. The atoms are usually arranged in giant regular lattices. Diamond and graphite are examples of giant covalent structures. In diamond, an allotrope of carbon, each carbon atom is covalently bonded to four other carbon atoms to form a giant covalent structure in which all the bonds are equally strong. Graphite, also an allotrope of carbon, has very strong bonds to three other carbon atoms giving layers of hexagonal rings. There is an electrostatic attraction between the layers as a result of the presence of delocalized electrons. These bonds between the layers are weak and the layers can slide over each other. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

The physical properties of giant covalent structures are due to their specific structures. Diamond is hard, has an extremely high melting point and does not conduct electricity. The former two properties are due to the strong bonds between carbon molecules and due to the absence of a plane of weakness. The latter property is due to the fact that diamond does not possess any delocalized electrons to carry a charge. Graphite on the other hand is soft and slippery, has a high melting point and conducts electricity. The soft and slippery property of graphite is due to its layers and their ability to slide over each other. The high melting point of graphite is because of the strong covalent bonds between carbon atoms. Finally, the conductivity of graphite is due to the delocalized electrons found between the layers. Figure 7 below displays the structure of diamond and graphite as illustrated in textbooks. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)



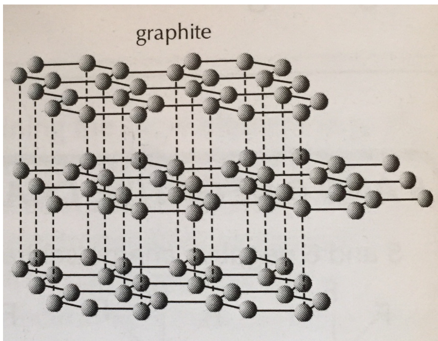


Figure 7: the structure of diamond and graphite (Neuss, 2007)

3.1.3 Metallic bonding

Metals form giant structures in which valence electrons of the metal are free to move. The valence electrons detach from individual atoms; hence, metals consist of a close packed lattice structures of positive ions in a sea of delocalized electrons. Metallic bonding is the electrostatic attraction between the positive ions and the delocalized electrons. Figure 8 below is a model of the bonding structure of gold (the yellow balls being the cations and the black ones being the delocalized electrons). (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

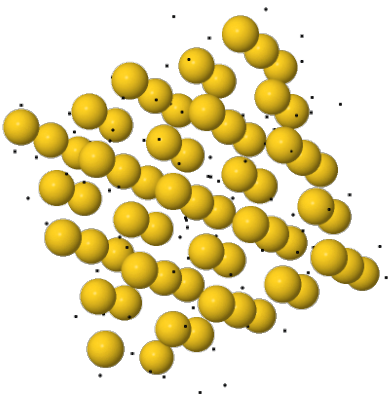


Figure 8: Metallic bonding in gold

Most metals have distinct properties, although, the extent of their properties differs depending on the metal. For example, some metals are better conductors of electricity then others. Metals are malleable and ductile, have high boiling and melting points, and they conduct electricity. Metals are malleable and ductile because the close packed layers of positive ions can slide over each other without breaking more bonds than are made. Metals have high melting and boiling points because the strong electrostatic attraction between the positive ions and the delocalized electrons are hard to overcome. Finally, metals conduct electricity due to the presence of the delocalized electrons that carry the charge. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

3.1.4 Similarities between ionic, covalent and polar covalent bonding

Generally, it is possible to predict if a compound has ionic or covalent bonds based on the difference in electronegativity. Usually if the difference in electronegativity between the two atoms is greater than 1,8 then the bond is ionic, otherwise it is covalent. However, there are many exceptions to the mentioned rule and often compounds are somewhere in between ionic and covalent. In reality these two bonding types are merely modifications of a similar pattern. Both types of bonding result from the electrostatic attractions between the electrons and protons of the atoms. Covalent and ionic bonding can be considered as a continuous pattern of bonding rather than a dichotomy. The difference merely being in the electron distribution. Figure 9 below portrays a visualization of ionic, polar covalent and covalent bonds respectively, with the molecular electrostatic potential (MEP) displayed. (Taber, 2001a; Taber & Coll, 2002; Kirouac & Consiglio)

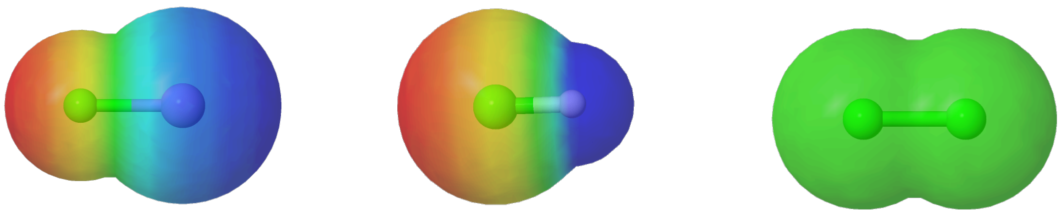


Figure 9: Molecular structure and MEP visualization of NaCl, HCl, and Cl_2 respectively

3.1.5 Relative Bond Length

Bond length is the average distance between the centres of the nuclei of two bonded atoms in a molecule. The shorter the bond length is, the larger the bond energy. It is measured in Angstrom units (Å) or picometers (pm). The bond length between two atoms depends on the size of the atoms. The smaller the atoms are, the shorter the bond length will be. This is because as the atoms get larger the distance between the protons of one atom and the electrons of the other atom gets larger. Hence the electrostatic attraction gets weaker, resulting in a weaker bond with a longer bond length. Additionally, the higher the bond order (number of chemical bonds between a pair of atoms) is, the shorter the bond length will be. This is because, the higher the bond order is, the stronger the bond will be and hence the shorter the bond length will be. (Brady & Senese, 2004; Neuss, 2007; Nivaldo, 2011)

3.2 Teaching Chemical Bonding

Bonding is a central concept in chemistry education; therefore, a thorough understanding of it is essential in order to understand various other topics in chemistry such as carbon compounds, proteins, polymers, acids and bases, chemical energy, and thermodynamics (Fensham, 1975; Gillespie, 1997; Hurst, 2002). Bonding is also the key to molecular structure and structure is closely related to the physical and chemical properties of compounds (Haluk Özmen, 2004). However, according to literature, bonding is considered to be a very complex concept, that students find difficult to understand (Gabel, 1996, Levy Nahum, Mamlok-Naaman, Hofstein, & krajcik, 2007; Robinson, 2003; Taber, 1998, 2001, 2002a; Tsaparils, 1997).

Chemists use a wide range of complex and sophisticated scientific models to make sense of chemical bonding. Learners are expected to develop an understanding of bonding through these diverse models and are additionally expected to be able to interpret a wide range of symbolic representations of chemical bonds. This is one of the reasons why learners find the concept of bonding difficult. Models, symbols and explanations of bonding, need to be both simplistic and authentic representations of scientific concepts and models in order to ensure that learners acquire a meaningful understanding of bonding. (Taber & Coll, 2002; Levy, Nahum, Mamlok-Naaman, Hofstein & Taber, 2010).

Students' live and operate within the macroscopic world and thus find it difficult to shift between macroscopic and molecular levels (Gabel, 1996; Harrison & Treagust, 2000, Johnstone, 1991; Robinson, 2003). Thus, understandably they tend to build alternative conceptions about bonding. However, according to Taber & Coll (2002), most alternative conceptions in chemistry are not resulting from the learner's informal experiences of the world but from prior science teaching. Students' alternative conceptions that largely stem from the way they have been taught, has been labelled by Taber (2001) as pedagogical learning impediments. In order to avoid pedagogical learning impediments being aware of common misconceptions among students and possible productive methods of dealing with the misconceptions is highly essential. The first sub chapters that follows describes the common misconceptions that students develop regarding bonding, which have been found in various previous researches. The second sub chapter that follows reports suggestions given to teachers on how to teach bonding, the suggestions are also based on findings from previous researches.

3.2.1 Common Student Misconceptions in Bonding

Through out the past two decades many researches conducted worldwide have documented numerous misconceptions/alternative conceptions that students develop regarding bonding. This sub chapter describes the misconceptions/alternative conceptions related to the 'octet' rule, ionic bonding, covalent bonding, covalent verses ionic bonding, metallic bonding, and intramolecular & intermolecular bonding.

The Octet Rule

According to research conducted by Taber & Coll (2002), by the age of 16 students commonly explain chemical processes with reasoning such as 'atoms want to have octets' or that 'atoms need to have full outer shells'. Often implying that chemical processes occur to allow atoms to achieve this. The focus that many teachers and textbooks place on the octet rule often results in learning impediments. Consequently, some students have difficulties accepting bonding which doesn't lead to atoms that have a full outer shells of electrons. Hence, intermolecular bonding, metallic bonds etc. seem mysterious to them. The octet rule is not an explanation for bond formation. Hurst (2002) refers to the octet rule as an oversimplification of the electronic structure of molecules. And according to Taber (2005), oversimplifications have the potential to act as significant impediments for future learning. (Taber & Coll, 2002; Levy Nahum, Mamlok-Naaman, & Hofstein, 2007; Levy Nahum, Mamlok-Naaman, & Hofstein, 2008)

Students reliance on the octet rule as an explanation for bond formation, leads them to acquire an 'atomic ontology'. In other words, students consider all molecular level species to derive from and comprise of atoms. Hence, learners view all starting material of chemical processes as being single unbounded atoms, which is hardly ever the case. The notion that 'everything is made up of atoms' helps confirm and justify their misconception. (Taber & Coll, 2002).

The octet rule also affects the way learners make sense of abstract chemical processes by using anthropomorphic language (Coll & Taylor, 2001a, 2001b; Taber, 1998, Taber and Watts, 2000). Students start using language that applies to psychological states and social situations to explain chemistry. Atoms are said to own, donate, accept, and to share electrons. They are also said to desire, need, want electrons and find themselves in a state of 'happiness' when they have a full outer shells or octets of electrons. Students have also used extreme language, such as, atoms being 'jealous' (Taber & Watts, 1996). Although most students are clearly aware that atoms are not living conscious entities, anthropomorphic explanations of the formation of chemical bonds inhibits them from acquiring a meaningful and accurate explanation of why bonds are formed. (Taber & Coll, 2002).

Ionic Bonding

Traditionally covalent bonding has been taught before ionic bonding. According to research, having studied covalent bonding first students often find it difficult to progress beyond the idea of covalent bonding. Hence with the concept of covalent bonding fresh in their minds, students tend to consider NaCl ion-pairs within the lattice as if they were molecules (by actually using this term). Research conducted by Levy Nahum, Mamlok-Naaman, & Hofstein (2008) suggests teaching ionic bonding before covalent bonding in order to assist students in grasping the concept correctly. Additionally, the fact that teachers often use ball and stick models to display ionic lattices may be instrumental in generating the misconception, since the sticks could possibly be mistaken for individual chemical bonds. (Taber & Coll, 2002; Levy Nahum, Mamlok-Naaman, & Hofstein 2008; Haluk, 2004).

Students tend to have little understanding of the electrostatic nature of chemical bonding (Boo, 1998; de Posada, 1997). Some students have been known to think of the attraction between two oppositely charge species to result in neutralization rather than bond formation (Boo, 1998; schmidt, 1997).

Covalent Bonding

Students commonly find it difficult to progress beyond the notion of 'shared pair of electrons', they tend to see it as something more than a metaphor (Taber, 2001a). Many learners see the shared electron pair as the bond, an idea that lacks explanatory power (Taber & Watts, 2000). Students have also been known to view the electron pair as something that holds the atoms together because it enables them to have octets of electrons. (Taber & Coll, 2002).

Scientifically, some covalently bonded materials exist in the form of molecules while others exist as covalently bonded lattices, such as diamond. Yet research suggests that learners do not fully grasp such structural diversity. (Taber & Coll, 2002).

Covalent verses Ionic

Typically, covalent and ionic bonds are taught as dichotomous 'electron sharing' or 'electron transferring' bonds respectively (Levy Nahum, Mamlok-Naaman, & Hofstein 2008). The difference in electronegativity between atoms is then used to differentiate ionic bonds from covalent bonds. However, bonds aren't always purely covalent or purely ionic. If at all purely ionic bonds don't actually exist at all. (Raymond, Peterson, & Treagust, (1989); Levy Nahum, Mamlok-Naaman, & Hofstein 2008)

Bonding should be described as intermediate, with varying degrees of ionic and covalent (and metallic) characteristics (Taber & Coll, 2002). Bond polarity is an indication of why covalent-ionic dimensions should be seen as a continuum rather than a dichotomy (Taber & Coll, 2002). However, research suggest that students tend to view bond polarity as an additional characteristic of covalent bonds, rather than as something between covalent and ionic (Taber, 2001a). This unfortunately leads some students to believe that polar substances such as hydrogen chloride exists as molecules in aqueous solutions (Barker & Millar, 2000).

Bond polarity can be explained based on electronegativity, which can be explained in terms of electrostatic attractions. However, electronegativity is only discussed in context of covalent bonding and not as an integral part of bonding polarity concepts (Weinhold & Landis, 2005). Hence, students often find it difficult to grasp the concept resulting in various misconceptions such as the view that non-polar molecules are formed between atoms of similar electronegativity or that ionic charge determines molecular polarity (Boo, 1998; Harrison & Treagust, 1996).

Metallic Bonding

Students often consider ionic and covalent bonding to be the only 'proper chemical bonds', hence assuming everything else to be 'just forces' (Taber & Coll, 2002). Some of the misconceptions regarding metallic bonding that have been discovered are: there is no bonding in metals; there is some form of bonding in metals, but not proper chemical boding; metals have covalent and/or ionic bonding; metals have metallic bonding, which is a sea of electrons

(Taber, 2001a). As discussed earlier for many students chemical bonding means atoms acquiring an octet of electrons in their outer shells. Hence some students find it difficult to understand the concept of metallic bonding and often assume that there is no bonding in pure metals, or that there is a 'lesser' form of bonding that is just a force and not a chemical bond. (Taber & Coll, 2002; Coll & Taylor, 2001a)

Many teachers and general chemistry textbooks introduce metals to have a set of common physical and chemical properties, such as, malleability, ductility, conductivity, etc. However, not all metals have common chemical properties, there is always some variability in the extent of these properties, for example, extent of brittleness, conductivity, boiling points etc. differs depending on the specific metal being discussed. (Levy Nahum, Mamlok-Naaman, & Hofstein 2008; Nahum et al., 2010)

Intermolecular and Intramolecular Bonding

Intermolecular forces are a key to chemical and biological behaviour and function (Gottschalk & Venkataraman, 2014). Understanding intermolecular forces facilitates an understanding of the importance of molecular-scale interactions and how they influence macro-scale observations. Additionally, thinking of intermolecular forces encourages students to predict various physical properties of compounds, such as boiling points, states of matter etc. However, many students tend to confuse intramolecular bonds and intermolecular bonds (taagepera et al., 2002). When students believe that intermolecular forces are interactions within molecules it affects their perception of phase change as well. For example, having learnt that water has a relatively high boiling point because of the presence of hydrogen bonds as intermolecular forces, it is quite natural that students conclude that in order for the phase to change actual covalent bonds must be broken. (Gottschalk & Venkataraman, 2014; Schmidt, Kaufmann, & Treagust, 2009; Cooper, Williams, & Underwood, 2015)

As discussed earlier, students tend to find it difficult to discuss any type of bonding that is not clearly explicable in terms of the octet rule. Since intermolecular forces such as hydrogen bonding and Van der Waals forces cannot be explained in terms of the octet rule, the difference between intermolecular and intramolecular bonding becomes blurry for many students. Additionally, when students do acknowledge intermolecular bonding they may not realize the distinction from covalent bonds (Pereira & Pestana, 1991). (Taber and coll, 2002)

3.2.2 Recommendations for Teachers

Students tend to have a wide variety of misconceptions regarding chemical bonding, the misconceptions relevant to this thesis were discussed in the chapter 3.2.1. Taber & Coll (2002) discuss various recommendations and suggestions for teachers regarding how to change the teaching of this topic in order to enhance student understanding and inhibit student's development of alternative conceptions. This chapter presents a description of the various suggestions of Taber & Coll (2002) and a few other educational researchers. Researchers suggest to focus on molecules and Ions rather than atoms. To teach bonding as an electrical concept (not a magical or social concept). To encourage teachers to emphasize the non-molecular nature of non-molecular lattices. They also suggest to 'take care with language'. And finally, they suggest to build on the physical principles and properties when teaching bonding.

Students atomic ontologies act as serious learning impediments which is why research suggest that teachers avoid talking about atoms in relation to bonding. Teachers are encouraged to focus on molecules and ions rather than atoms, on how molecules and ions behave rather than on how they are formed. How molecules or ions came into being is of no relevance in bonding. Once bonding is perceived as primarily driven by electrical forces, there will be no need to explain it in terms magical or social concepts. Chemical bonds should be understood as physical forces holding together chemical systems such as lattices and molecules. Bonds hold molecules together by electrostatic attractions both within molecules and between molecules. (Taber & Coll, 2002; Levy Nahum, Mamlok-Naaman, & Hofstein 2007, 2008; Nahum, et al. 2010)

However, once students have been taught about molecules, they then have a tendency to view all bonding structures as such. Hence once the topic of metallic bonding approaches they may view metals as individual molecules of similar atoms similar to iodine or phosphorus. Hence it is necessary to emphasise the non-molecular nature of metallic bonding. (Taber & Coll, 2002)

Teachers are also recommended to be extremely careful with their use of language. Shifting from everyday terminology to theoretical molecular levels of description will always be central in chemistry teaching. Therefore, it is important to model the way chemists use molecular notions to explain macroscopic phenomena. We must, for example, be careful and make sure substances and not molecules are said to evaporate, melt, expand etc. Additionally, using anthropomorphic and other metaphorical language to explain concepts must be carefully considered as well. It is important that students to do not assume molecular interactions are like social interactions and can be explained in terms of physiological needs and wants. It is also necessary to make sure that such descriptions are mere anchors for more scientific descriptions and explanations. (Taber, 2002; Taber & Coll, 2002)

Finally, when teaching bonding it is essential not to make assumptions regarding students understanding. It is important to specify underlying principles, without assuming that students are aware of the physical forces involved. Teaching bonding often unnecessarily emphasises processes, such as, hypothetical schemes for bond formation, and sadly places little importance on the outcomes of bonding. This is highly unproductive as all scientists aim to use bonding to explain properties and predict reactivity. Having covered the concepts of bonding and the underlying physical principles, teachers are encouraged to facilitate the connection between the sub-microscopic and the macroscopic levels. This could be achieved by building on physical properties and phenomena of material with respect to bonding and structure. It is important that students are able to truly understand the link between bonding and the various physical properties that result from it. (Levy Nahum, Mamlok-Naaman, & Hofstein 2008; Taber & Coll, 2002)

Table 1 below highlights the above presented ideas teachers should take into account when teaching the various types of bonding.

Table 1: Ideas for teaching bonding

Type of bonding	Ideas
Ionic bonding	• Base explanations on electrical forces/attractions • Promote effective transitions between macroscopic and molecular levels (properties) • Ionic and covalent bonding should be seen as a continuum rather than a dichotomy • Focus on molecules and ions rather than atoms. Not on how ions are formed but on how they behave • Build on physical properties • Avoid discussing psychological needs/wants • Emphasise that electronegativity is not a definite method of differentiating between ionic and covalent bonds • Present students with diverse models
Covalent bonding	The above presented ideas for ionic bonding also apply to covalent bonding, including the following ideas: • Emphasise that electrons are not always shared equally in covalent bonding • Make sure the octet rule does not inhibit students understanding of bonding • Discuss similar patterns of bonding between ionic and covalent
Dipole-dipole bonding	• Base explanations on electrical forces • Focus on the relationship between intermolecular forces and physical properties • Build on physical properties • Highlight the importance of intermolecular forces • Discuss relative strength of the diverse types of bonding • Polarity should be introduced as something between covalent and ionic bonding rather than a secondary characteristic • Highlight that hydrogen bonding is not the bonding of hydrogen with other atoms • Students must be introduced to real life situations related to hydrogen bonding
Van der Waals forces	• Base explanations on electrical forces • Focus on the relationship between intermolecular forces and physical properties • Build on physical properties • Highlight the importance of intermolecular forces • Discuss relative strength of the diverse types of bonding
Metallic bonding	• Base explanations on electrical forces/attractions • Promote effective transitions between macroscopic and molecular levels (properties) • Build on physical properties • Avoid discussing psychological needs/wants • Emphasize that metallic bonding is 'proper chemical bonding' • If using the analogy 'metallic bonding is a sea of electrons', make sure students truly understand the concept

4. Computer-based Molecular Models

This chapter introduces molecular models and their importance in chemistry and chemistry education. After which, the uses of computer-based molecular modelling in education are presented, together with the useful features of computer-based molecular modelling software. Then finally, the challenges of using computer-based molecular modelling to enhance learning are discussed.

4.1 Molecular Models and Computer-based Molecular Models

Although it is probable that chemical ideas have been visually, mathematically or verbally modelled since they began to be produced; the first concrete models for atoms was produced by John Dalton at the beginning of the nineteenth century. Thereafter, leading chemists, for example, Kekule, Van't Hoff, Pauling, Watson and Crick have used models to present, develop, and discuss ideas regarding molecular structures. The use of models helped with their predictions of the behaviour of substances, and supported their ideas regarding structure. Hence, molecular models became highly crucial tools in the study of stereochemistry, properties, and reactivity of substances which, in turn, corroborated the atomic theory (Francoeur, 1997). (Justi & Gilbert, 2002)

"A model is a readily perceptible entity by means of which the abstractions of a theory may be brought to bear on some aspects of the world-as-experienced in an attempt to understand it" (Gilbert et al. 2000, p. 34). There are two types of models: mental models and material models. Mental models are representations that we build in order to explain or predict a situation, they are often "forerunners of misconceptions" (Kind, 2004). Mental models are created in the moment when they are needed and are then discarded when they are no longer needed. Material models are expressed mental models (Gilbert et al., 2000) that are built to communicate with other individuals. Material models can be symbolic, experimental, or iconic. Figure 10 below represents the relationship between the real world, mental models and material models (symbolic, experimental or iconic) according to Chamizo (2011).

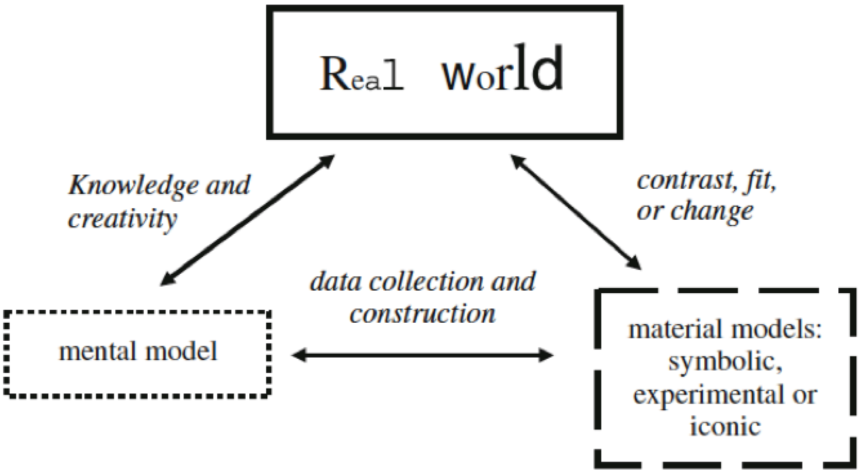


Figure 10: The relationship between the real world, the two types of models and modelling (Chamizo, 2011)

Molecular models, real or computer-based, are highly productive tools that facilitate visualizing chemistry. Visualizations help externalise thought, facilitate memory, information processing, collaboration and other activities (Jones et al., 2005). Molecular models could be used at all levels of education as teaching aids since modelling is a highly essential tool to understand chemistry, few of the macroscopic observations can be understood without the aid of sub-microscopic representations or models (Oversby, 2000). Learning chemistry involves: (i) getting acquainted with major models produced by chemists, as well as understanding the scope and limitations of such models; (ii) appreciating the role of models in developing and presenting the products of chemical enquiry; and (iii) building and testing chemical models produced by individuals and/or groups (Justi & Gilbert, in press a). Hence, a complete understanding of models and modelling is crucial for students' productive learning of chemistry. (Aksela & Lundell, 2008; Justi & Gilbert, 2002)

The use of modern computer-based molecular modelling has proven to be highly productive in chemical research (Justi & Gilbert, 2002). Computer-based molecular modelling opens various possibilities for teaching chemistry (Aksela & Lundell, 2008). Barak and Dori (2005) found that using computer-based models helped promote students' understanding of chemistry at four levels: the macroscopic, microscopic, symbolic and chemical process levels. They also found that computer based visual models helped students understand chemical concepts, theories, and molecular structures. Additionally, Ardac and Akaygun (2005) found that students who studied molecular representations and the structure of matter with the use of computer-based models outperformed their peers who didn't use computer-based models.

4.2 Uses of Computer-based Molecular Modelling in Education

Computer-based molecular modelling has been used for illustrating models and concepts in chemistry, and has been found to revitalise and diversify teaching (Feller et al., 2004; Hessley, 2004; Tasker and Dalton, 2006). Computer-based molecular modelling could be used to facilitate students understanding of the diversity of models and their limitations. It could also assist students in making efficient transitions between the macroscopic and molecular levels. Additionally, computer-based molecular modelling could be used by teachers for demonstrations or by students for inquiry. Finally, it could also be used to enhance student's visualization of abstract concepts. Computer-based molecular modelling software have various features that support it as a highly effective learning tool.

In chemistry, models are mere enlargements of the molecules they are intended to represent. This explains the multiplicity of models that can be used to represent the same molecule. Unfortunately, teachers often use one type of model to represent the same molecule; thereby, eliminating student acquaintance with the diversity of other models. This leaves students with only a partial grasp of the model or a complete misunderstanding of it. Therefore, it is important to discuss various models, while recognizing their limitations. Computer-based molecular modelling provides teachers with a highly efficient method of presenting students with diverse models of the same molecule. Computer-based molecular modelling could also be used as a tool to introduce students to the nature of a model. It is also important that students understand that models are not scaled (Hardwicke, 1995). For it is only by understanding that models are analogies with different scopes and limitations that students will be able to productively use them to explain, predict and understand the diverse properties of substances. (Justi & Gilbert, 2002; Barnea & Dori, 2000; Boulter & Gilbert, 2000; Frailich, Kesner, & Hofstein, 2008; Drechsler, 2007))

Students misconceptions are often a result of the fact that they live and operate in a macroscopic world of matter and hence do not easily follow shifts between the macroscopic and sub-microscopic levels (Gabel, 1996; Harrison & Treagust, 2000). Computer-based models help students make effective connections between their macroscopic worlds and the sub-microscopic level (Frailich, Kesner, & Hofstein, 2008).

Computer- based molecular models could be used by teachers during lectures (as demonstrations), freeing teachers from the limits that drawing on the board imposes. The use of computer-based molecular models could allow for representation of more accurate models. Teachers could also use it as a tool to liven discussions and encourage students to think for themselves. Computer-based molecular modelling could also be used by students in an activity to investigate and inquire. Regardless of how computer based modelling is used in the classroom it motivates students and promotes their interest in chemistry. (Hehre & Shusterman, 2000; Aksela & Lundell, 2008).

Studies of student's (and sometimes expert's) use of computer-based molecular models indicate that they could improve visualization in chemistry (Barnes, 2000; Ealy, 1999; Fleming et al, 2000). Computer-based molecular models facilitate the visualization of abstract entities and provide a basis for scientific thinking. For example, computer-based molecular modelling illustrates strong and weak bonds well through partial charge distribution. (Aksela & Lundell, 2008; Justi & Gilbert, 2002)

Useful Features of Computer-based Molecular Modelling

There are several useful features that many computer-based molecular modelling software provide to facilitate the understanding of chemical bonding. For example, it is possible to view several models of the same molecule (wire, tube, ball and stick, space filling, and dot surface) with just one click. The importance of being able to view various models of the same molecule has already been highlighted above. It is also possible to view the hydrogen bonds between molecules such as water molecules. This is also a highly useful feature, because it enables students to visualize the electrostatic attractions. Measuring the bond length is an additional feature that enables students to investigate for example the relation of bond length to bond order. Finally, a highly productive feature available in many molecular modelling software, such as Edumol, is the ability to visualize the molecular electrostatic potential (MEP) maps. Molecular electrostatic potential can be mapped onto the electron density by using colour to represent the value of the potential. The model thus illustrates simultaneously molecular size and shape and the electrostatic potential. Hence the maps allow one to visualize variably charged regions of molecules. Colours closer to red indicate negative partial charges, while colours closer to blue indicate positive partial charges. (Hehre & Shusterman, 2000; Shusterman & Shusterman, 1997)

4.3 Challenges of Using Computer-based Molecular Modelling as a Learning Tool

There have been a couple of researches (Feller et al., 2004; Hessley, 2004; Tasker; Dalton, 2006; Frailich, Kesner, & Hofstein, 2008; Drechsler, 2007; and Hehre & Shusterman, 2000) conducted that have examined the usefulness of computer-based molecular modelling as a teaching tool. There have also been researches (Aksela & Lundell, 2008) conducted that have examined using computer-based molecular modelling for teaching from a teachers' perspective, analysing the factors that inhibit/enhance teachers use of computer-based molecular modelling in the classroom. However, there is a lack of researches conducted that have examined the challenges of using computer-based molecular modelling as a learning tool from a student's perspective. The research conducted for this thesis examines the challenges students face when using computer-based molecular modelling as a learning tool and how to optimally support students.

5. Design Product

The entire design process comprised of designing the exercise questions, the models for visualization and the questionnaire. This chapter first presents a brief description of each question and model used in the exercise, followed by an explanation of the objectives of each question and model. The chapter then presents suggestions for implementing the exercise during a lesson. After which, an explanation is given for the design of the questionnaire.

5.1 The Modelling Exercise and the Models

The exercise was designed taking into consideration suggestions on how to teach bonding from previous researches. The exercise provides students with brief explanations/descriptions of the type of bonding being discussed, after which, it outlines the molecules and properties that need to be visualized. Having read the brief explanation and visualizing the molecules and properties, students are then expected to answer various questions. The exercise goes through the following topics consecutively: Ionic bonds, Simple Covalent compounds (Dipole-diploe forces, hydrogen bonding, and Van der Waals Forces), Giant Covalent compounds, Metallic bonds, Similarities between ionic, covalent and polar covalent bonding, and bond length. The subchapters that follow briefly describe the questions posed and the models presented within each topic. The subchapters also provide the objective or rationale of the question posed and the model visualized. The initial design of the exercise can be found in appendix 1 and the files for the models can be found in appendix 4.

5.1.1 Ionic Bonding

This section consists of two main questions. In order to answer the questions, students need to visualize in Edumol, three dimensionally the models presented in figure 11 below.

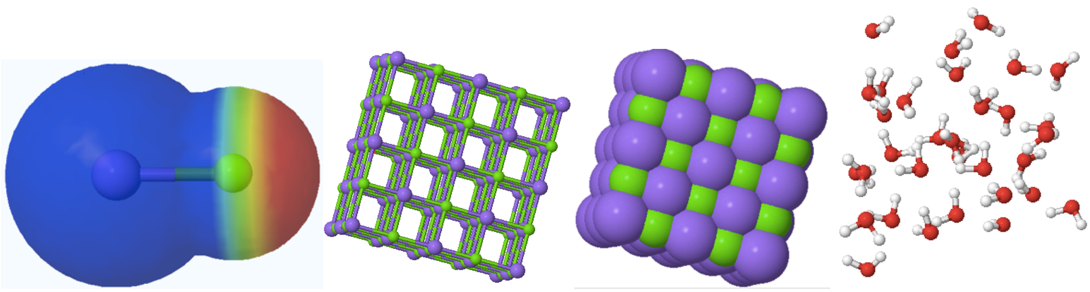


Figure 11: Models of NaCl, Salt crystal, Salt crystal (space filling model) and water

The first question of this section explains the formation of sodium chloride and the various steps involved in the formation of sodium chloride. It also describes the relative amount of energy consumed or released at each step. The question then asks students to explain ‘based on electrical forces’ why the formation of sodium chloride is an exothermic reaction.

The question is designed to encourage students to think of ionic bonding in terms of electrical forces/attractions rather than focusing on the formation of ions. The idea behind mentioning electrical forces is to further emphasise/encourage students to use it as a means of explaining bonding rather than focusing on psychological needs and wants. Additionally, the visualization of the salt crystal is meant to support students understanding of lattice structures and to promote understanding of the fact that numerous ions are joined together in the formation of lattice structures. Finally, the presentation of the CPK (space filling) model of the salt crystal is to enhance students understanding of ionic bonding, by attempting to eliminate any possible misconception that the ball and stick model might support (the sticks being mistaken for individual chemical bonds).

The second question focuses on the distinct properties of ionic structures. One of the main objectives of this question is to promote student’s ability to make effective transitions between macroscopic and molecular levels. Another aim is to encourage students to build their knowledge of bonding on the physical properties of materials.

Part a and b of the second question conveys that aqueous solutions conduct electricity in water and that ionic compounds are soluble in polar solvents. Students are then supposed to draw their own models of a sodium chloride aqueous solution based on the visualized models of salt and water. They are also supposed to explain their models describing why aqueous solutions conduct electricity. Part c of the second question mentions that ionic crystals are relatively hard but brittle, students are supposed to visualize the CPK model of the salt crystal and explain why they are brittle. The idea in part c is that students visualize how hitting a spoon or knife on one part of the crystal could shift the position of the crystals possibly causing like charges to come into contact and repel each other. Part d of the second question mentions the high boiling and melting points of ionic compounds, asking students to explain this. In part d, students should be able to explain the property based on the strong bonds of lattice structures. Finally, part e of the second question reveals the low volatility of ionic compounds asking students to explain once again based on the structure of ionic lattices.

5.1.2 Covalent compounds

The covalent compounds section consists of Simple Covalent Compounds and Giant Covalent Structures. The simple covalent compounds section further includes the types intermolecular bonding present between simple covalent compounds, dipole-dipole forces and Van der Waals forces.

Simple Covalent Compounds

The third question briefly explains covalent bonding. Students are then required to visualize HCl and Cl_2 three dimensionally in Edumol. They are also encouraged to visualize the molecular electrostatic potential (MEP) of the mentioned molecules. Figure 12 below portrays a 2D representation of the models.

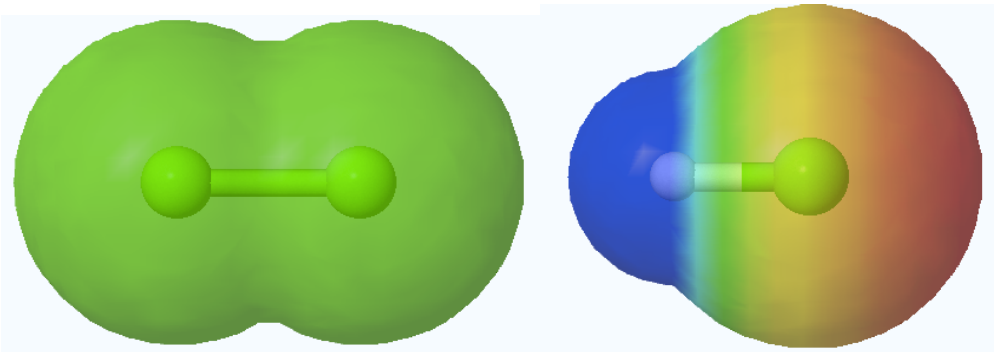


Figure 12: Models of Cl_2 and HCl displaying MEP

After visualizing the above, students are then required to explain the electron distribution of Cl_2 and HCl based on the visualization. Students are also asked to explain why HCl is a polar covalent compound and Cl_2 a non-polar covalent compound. The objectives of using these particular questions and models is to persuade students to consider bonding that is an intermediate between ionic and covalent. It also aims to eliminate misconceptions that "electrons are shared equally in covalent bonds". Additionally, it aims to focus on the electrical attractions between molecules as an explanation for bonding. Finally, it is an attempt to discourage students from viewing polar covalent bonding as a secondary characteristic of covalent bonding rather than something between covalent and ionic.

The exercise then explains the difference between intermolecular forces and intramolecular bonding, seeking to clarify the difference at this point in order to eliminate pre/mis conceptions student may have developed. The brief explanation classifies intermolecular forces as attractions **between** covalently bonded molecules. Presenting dipole-dipole (including hydrogen bonding) intermolecular forces and Van der Waals forces (dispersion) intermolecular forces. Intramolecular forces are then described as attractions **within** covalently bonded molecules.

Dipole-dipole forces (intermolecular forces)

After explaining the existence of permanent dipole moments in polar molecules (as a result of polar covalent bonds), students are required to visualize an ICl molecule three dimensionally in Edumol, also visualizing the MEP. An image of the mentioned visualization is displayed in figure 13 below.

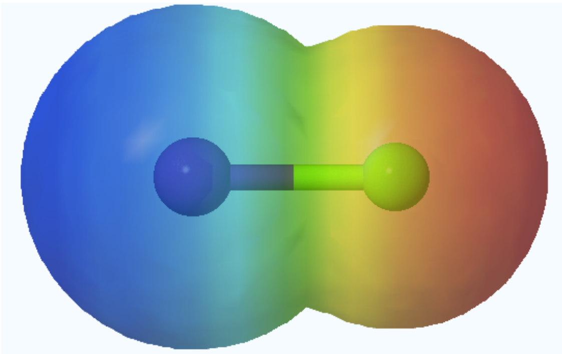


Figure 13: Model of ICl displaying MEP

The fourth question then asks students to draw the intermolecular forces between three ICl molecules and explain the electrostatic attractions. This question aims to support students understanding of intermolecular forces further, allowing students to focus on the attractive forces between polar covalent compounds. The model promotes understanding of partial charges; hence, further fostering focus on electrical attractions.

After an explanation of hydrogen bonding, question five asks students to visualize three dimensionally hydrogen bonding in water and ice via Edumol. An image of the visualization is displayed in figure 14 below. The objective of the visualization is to eliminate the possible misconception that a hydrogen bond is a covalent bond to hydrogen. The visualization could also reinforce the concept of intermolecular bonding. Additionally, it allows students to analyse the difference in the structure between ice and water.

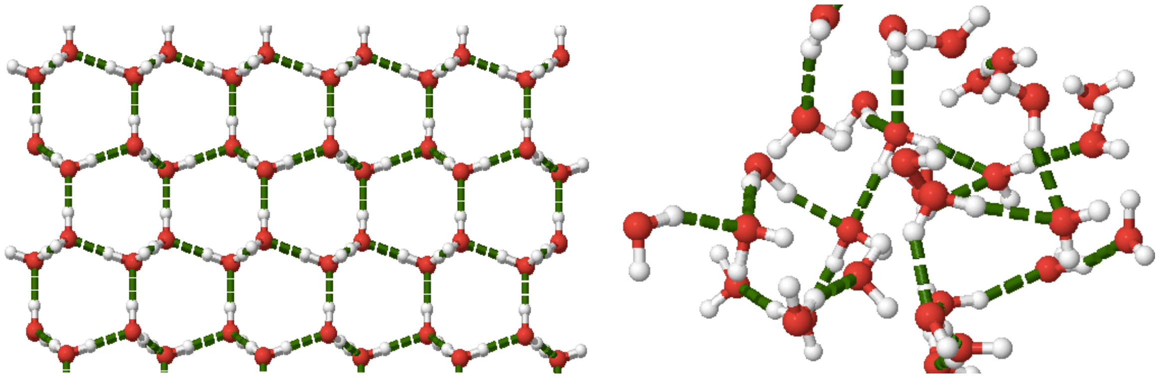


Figure 14: Models of ice and water with visualizations of the hydrogen bonds between the H_2O molecules

The sixth question requires students to use the knowledge acquired thus far to "answer what factors affect the strength of dipole-dipole bonding?". The objective of this question is to facilitate students understanding of partial charges and polar covalent compounds. Additionally, the question aims to further enforce the concept of an intermediate between covalent and ionic bonds.

Van der Waals Forces (Intermolecular forces)

After explaining the existence of temporary (instantaneous) dipoles in non-polar covalent molecules, an image illustrating an induced dipole of a Helium atom is presented in the exercise. The image which was acquired from an article by Kirouac & Consiglio can be seen in figure 15 below. The reason for providing students with the two dimensional image is because it is impossible to visualize it three dimensionally in Edumol.

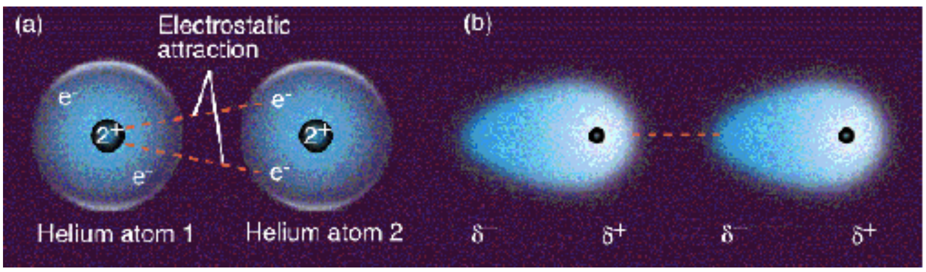


Figure 15: Induced dipole of a helium atom (Kirouac & Consiglio)

Question seven expects students to explain why Van der Waals forces increase with increasing mass. The objective of the question is to ensure that students understand how Van der Waals forces function.

The eighth question focuses on the distinct properties of simple covalent structures. One of the main objectives of this question is to prompt the practice of making effective transitions between macroscopic and molecular levels. Another objective is to encourage students to build their knowledge of bonding on the physical properties of materials.

For part a of the eighth question students are asked to explain based on electrostatic attractions why covalent compounds have low melting points, low boiling points and high volatility. Once again students are encouraged to explain bonding in terms of electrical attractions rather than in terms of 'physiological needs and wants'. Additionally, students are diverted towards making connections between the relative bond strengths. Hopefully at this point students will also begin to realize the importance of intermolecular forces. Then in part b students are required to explain based on electrical forces why covalent compounds do not conduct electricity. Part c requires students to then explain the solubility of three covalent compounds: ethane, ethanol, and heptanol. Students are encouraged to visualize the structures of the mentioned molecules as well as their MEP's in Edumol. The mentioned visualization can be seen in figure 16 below. The objective of the question is to prompt students to figure out and explain based on electrical attractions why ethane is insoluble in water, heptanol is very slightly soluble in water, and ethanol is soluble in water. The question aims to enhance student understanding of solubility, while facilitating the practice of making effective transitions between macroscopic and molecular levels.

Figure 16: Models of heptanol, ethane and ethanol respectively, displaying MEP

Giant Covalent Compounds

After being presented with an explanation of giant covalent structures, students are required to visualize models of diamond and graphite, paying particular attention to the delocalized electrons between the layers of graphite. Figure 17 below presents a two dimensional visualization of the structure of diamond and graphite.

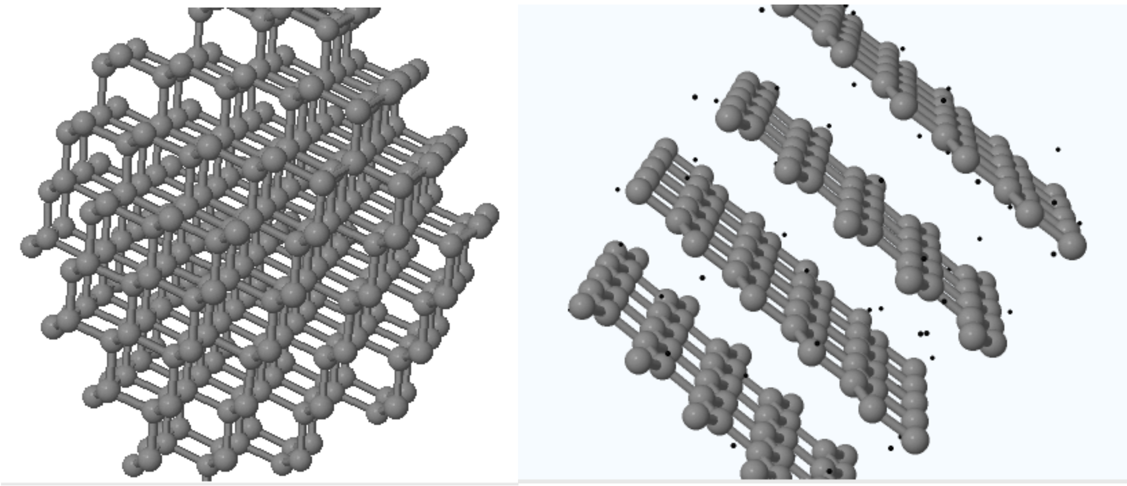


Figure 17: models of diamond and graphite

In part a of question nine students are required to explain based on the viewed models why graphite is soft and slippery, has a high melting point and conducts electricity. The aim is for students to realize graphite is slippery as a result of it's layers, it has a high melting point as a result of its giant structure and it conducts electricity due to the presence of delocalized electrons. Part b of question nine requires students to explain why diamond is hard, and has a very high melting point. The aim of this question is to ensure that students understand the nature of very strong giant covalent structure. Overall, the ninth question was designed to facilitate student understanding of the importance bonding at a macroscopic level.

5.1.3 Metallic Bonding

The tenth question requires students to view a three dimensional model of gold, in order to visualize an example of metallic bonding. Figure 18 below presents an image of the mentioned visualization.

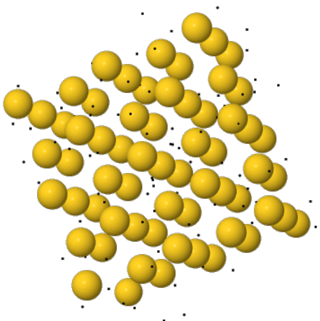


Figure 18: A model of gold, with visible delocalized (black dots).

After reading the explanation for metallic bonding and visualizing the model of gold, students are asked to explain metallic bonding in terms of electrical attractions. Once again students are encouraged to focus on electrical attractions when explaining bonding. The question intends to convey that metallic bonding is a form of proper chemical bonding. The objective of visualizing the model is to ensure that students form a clearer understanding of the analogy 'metallic bonding is a sea of electrons'.

Question eleven focuses on the distinct properties of metals. A brief explanation before the questions enforces the idea that not all metallic bonds are identical, they differ in the extent of the properties. For example, some metals are better conductors of electricity than others, even though all metals conduct electricity.

Part a of question nine requires students to explain based on the structure why metals are malleable and ductile. This question is meant to encourage students to think about how the closely packed layers of positive ions can slide over each other without breaking bonds. Part b of question nine requires students to explain based on the structure why metals have high melting and boiling points. Here once again the question aims to encourage students to use electrical attractions to explain. Finally, part c requires students to explain metals ability to conduct electricity. This question aims to reinforce the presence of delocalized electrons. Over all question nine aims to facilitate student's effective transitions between macroscopic and molecular levels, and to encourage students to build on physical properties of materials. Students are also encouraged to observe the importance of bonding and the effect it has on everything around us.

5.1.4 Similarities between ionic, covalent and polar covalent bonding

Students are first required to visualize models of NaCl, Cl_2, and HCl three dimensionally displaying MEP. An image of the representation can be seen in figure 19 below.

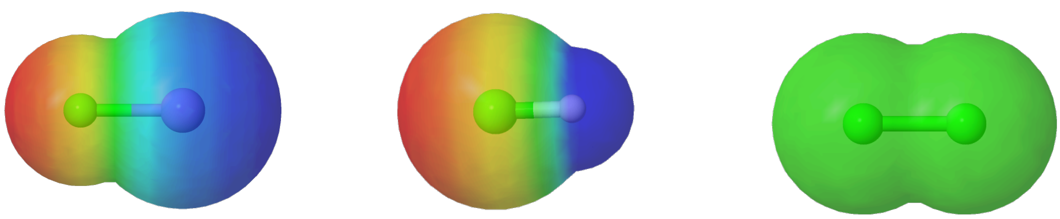


Figure 19: Models of NaCl, HCl, and Cl_2, additionally displaying MEP

In question twelve, students are first provided with an explanation of how ionic and covalent compounds differ from each other. They are additionally informed that the difference in electronegativity is no certain method to decide if a compound is ionic or covalent. Students are then encouraged to notice patterns between ionic, covalent and polar covalent bonding. Then finally, students are asked to explain why ionic and covalent bonding should **not** be viewed as a dichotomy. The aim is to reinforce the idea that ionic and covalent bonding have a similar pattern and that the main difference is in the distribution of electrons.

5.1.5 Bond length

The section begins with a definition of what bond length essentially means and its units of measurement.

Question thirteen requires students to discover a relation between bond length and the size of the bonded atoms. Students are encouraged to examine the bond length between F_2, Cl_2, and Br_2 to assist in their explanation. This can be done quite easily using Edumol, the molecules could be placed side by side and the length could be measured. Figure 20 below displays the models of F_2, Cl_2, and Br_2, consecutively, with the last model displaying the bond length of Cl_2.

Figure 20: Consecutive models of F_2, Cl_2, and Br_2, with the bond length of Cl_2 displayed

Question fourteen requires students to discover a relation between bond length and bond order. Students are encouraged to examine the bond lengths between the carbon atoms of ethane, ethene, and ethyne to assist them in their explanation. This can be done quite easily using Edumol, for example the molecules could be placed side by side and the length could be measured as seen in figure 21 below.

Figure 21: Consecutive models ethyne, ethene, and ethane.

5.2 Implementation during a Lesson

The exercise is designed to be used in parts rather than as a whole when implementing during a lesson. The research process required students to complete the entire exercise (14 questions) together, in order to create the concept maps. However, in a classroom situation, teachers must select the questions/sections according to the topics being taught. This chapter highlights main learning objectives of the design product as well as suggestion on how to implement it during a lesson.

5.1.1 Main Learning Objectives

The main learning objectives of the entire exercise include:

- To build knowledge of bonding on physical properties of materials
- To make effective transitions between macroscopic and molecular levels
- To differentiate between intermolecular and intramolecular bonding
- To explain bonding through electrical forces/attractions
- To demonstrate the significance of intermolecular bonding
- To focus on the relative strength of various types of bonding
- To reinforce that covalent bonding does not necessarily mean equal sharing of electrons
- To view ionic and covalent bonding as a continuum rather than a dichotomy
- To view polar covalent bonds as something between ionic and covalent rather than an additional character of covalent bonding
- To facilitate student's ability to apply their knowledge and to enhance evaluative and critical thinking.

The methods for achieving the above mentioned learning objectives are highlighted in chapter 5.1 as an explanation for the use of each question and model.

5.1.2 Suggestions for Implementation during a lesson

The exercise was initially designed to be implemented during a lesson as an inquiry exercise prior to teaching each section/topic or as a class exercise after teaching each section/topic. The idea being that students could read through the explanations and the questions, visualize the models in Edumol and then answer the questions in written form on paper/notebooks.

An advantage of requiring students to do the exercise prior to teaching the topic is that it promote students interest in the topic and facilitate their thinking skills. It could also promote their inquiry skills, which in turn would also enhance their understanding of bonding. Finally, doing the exercise prior to studying the topic could facilitate an understanding of bonding based on physical properties and assist students in making effective transitions between macroscopic and molecular levels.

Requiring students to do the exercise after the topic has been taught could also be advantageous. It could reinforce the concepts of bonding, ensuring that students remember the concepts taught to them. Additionally, it could help students focus on certain concepts that they might not have understood during the lecture. Finally, it could eliminate possible alternative conceptions formed during the lecture. Regardless of when the exercises are introduced, students will be able to view the models three dimensionally and make better sense of the abstract concepts of bonding.

5.3 The Questionnaire

The questionnaire (appendix 2) consists of seven questions, out of which four are open-ended questions, one is closed-ended and two are both. Closed-ended questions are questions where all possible answers are provided to the respondent. The advantages of closed-ended questions are that they provide clear cut answers, with little effort from the respondent. It is also easier to analyse closed-ended questions, as it eliminates the possibility of misinterpretations. Using closed ended questions is a highly efficient method of acquiring useful information from respondents that aren't motivated. However, the disadvantages of closed-ended questions are that sometimes respondents might feel that the answer is not very clear cut. Thus, if worded poorly, the question could frustrate respondents and provide inaccurate answers. On the other hand, open-ended questions are questions that allow respondents the freedom to answer according to their own desires. The advantages of using open-ended questions are that they provide flexibility, and possibly provide the respondent with the opportunity to illustrate their true opinions. However, the disadvantages of using open ended questions are that it could be highly time consuming to answer, it might be hard to analyse (leading to misinterpretation), and the answers provided by the respondent might not always answer the question asked.

The first question was both a closed-ended as well as an open-ended question requiring students to answer if they enjoyed the exercise with a yes, no or it was ok. They were additionally required to provide a reason for their answer. The second question was a closed-ended question for which students were required to answer if the exercise was too hard, too easy or just right. The third question was both an open-ended and a closed-ended question requiring students to answer whether the visualizations enhanced their understanding of chemical bonding, with a yes, no, or both yes and no. They were additionally required to provide a reason for their answer. The rest of the questions were all open-ended. The fourth question required students to tell what they liked most about the exercise, and to provide a reason for their answer. The fifth question required students to explain what aspects of the exercise promoted their understanding. The sixth question required students to reveal if they thought the exercise would be useful to use as a class activity when studying the topic. Finally, the seventh question required students to mention any changes they would like to make to the exercise, with an explanation as to why.

The main objective of the questionnaire was to prompt students to express their opinions regarding the explanations, questions and the models. The aim of the research was to acquire an insight into the challenges students face when using computer-based molecular modelling to comprehend bonding, and to acquire an insight into what students find useful. Hence; was highly essential to gather student's opinions and ideas, which is was the main objective of the questionnaire.

6. Data Analysis and Research Results

Research data was acquired mainly from the questionnaires and from observations which were acquired during the research process. Few ideas were gathered from the concept maps as well. The concept maps were analysed by evaluating the changes students made in their concept maps after doing the modelling exercises. The analysis of the questionnaire was conducted via thematic analysis. Chapter 6 first of all presents the data analysis method after which the research results are presented. Then the reliability of the results is discussed and finally, the improvements made based on research are discussed.

6.1 Data Analysis

As mentioned earlier the main source of data was the questionnaire. Additionally, the concept maps provided some information. Since the concept maps did not provide much data, the main analysis method used for it was merely a comparison between each students three concept maps. The questionnaires on the other hand were analysed more extensively. The questions from the questionnaires were divided into open ended and closed ended questions. The closed ended questions did not require a deep analysis as there were only three options that the students could chose from, and the results of those questions are directly presented in chapter 6.2. The open ended questions on the other hand required further analysis, the answers to the open ended questions were analysed using thematic analysis.

6.1.1 Thematic analysis

The research data was first analysed and categorized into main emerging themes, using sentences as coding units. The sentences in each category were then further coded to create sub categories. For example, a student mentioned *"I think it would do better as homework than class activity, because the procedure is quite individual. As homework it could be useful. In class I prefer learning methods that really make use of the teacher´s expertise rather than electronic devices"*. This response was first divided into two categories. The suggestion to use computer-based molecular modelling as homework was categorized as a supportive suggestion. The preference for using the teacher's expertise in class as a learning method rather than electronic devices, was categorized as one of the challenges encountered when using computer-based molecular modelling in class. The suggestion to use it as homework was then further categorized as a possible improvement to the ideas of implementation during a lesson.

And the preference for using the teacher's expertise in class rather than electronic devices was further categorized as one of the technical challenges. The resulting categories were then presented in the results as appropriate.

Thematic analysis is a method used to identify analyse and report themes within data. The word 'theme' refers to a specific pattern that is found in the data which is relevant to the research question. It facilitates organizing and describing research data in detail. For thematic analysis it is necessary to create conceptual tools to classify and understand the phenomena being studied. This involves analysing the complex and detailed data in order to find features that are crucial for the research. This is done by coding, which is a widely used term for categorising data. (Marks & Yardley, 2004; Braun & Clark, 2006; Tuckett, 2005; and Bowen, 2009)

Coding involves taking chunks of text and labelling them into various categories, so that one can later retrieve and analyse the data. The research questions determine what one choses to code from the data, since the codes must flow from the research question that require answering. The entire set of codes in a research consists of the coding frame. The coding frame allows one to systematically compare texts being analysed and it is through the frame that one is able to acquire answers from the data. (Marks & Yardley, 2004; Braun & Clark, 2006; Tuckett, 2005; and Bowen, 2009)

Coding involves finding patterns in data and dividing the data in order to create clarity. The unit of coding must be decided ahead of time. The unit for coding used in this research was sentences. The data was analysed and categorized in order to search for sentences that indicated what kind of challenges students encountered and what features supported their learning. The sentences of each category were then further coded. The sentences which indicated the kinds of challenges students encountered were further coded into challenges due to the research method and challenges due to the use of models. The challenges due to the use of models, were further coded into technical challenges, challenges related to prior use of models, and challenges related to student attitudes. The sentences which indicated features that supported the students learning, were then further categorized into supportive elements directly related to the models and modelling, and supportive elements related to the exercise. (Marks & Yardley, 2004; Braun & Clark, 2006; Tuckett, 2005; and Bowen, 2009)
Once all the data is categorized one can begin the analysis. The codes could be used in a quantitative manner; however, for this analysis the codes were used for a purely qualitative

analysis. In qualitative analyses the focus is on the description of verbal patterns. The codes were analysed in order to get answers to the research questions. The results which are based on the student's direct verbal descriptions are presented in chapter 6.2 below. (Marks & Yardley, 2004; Braun & Clark, 2006; Tuckett, 2005; and Bowen, 2009)

6.2 Results

The research results are grouped into three categories corresponding to the three main research questions (see chapter 2.2.2). The results are presented as follows: 1. Challenges of using computer-based molecular modelling in the classroom, 2. Some of the most useful features of computer-based molecular modelling, 3. Supporting student's usage of computer-based molecular modelling, and 4. Quantitative results presenting students opinions regarding the modelling exercise.

Challenges of using Computer-based Molecular Modelling in the Classrooms

Students seemed to have encountered many challenges while carrying out the modelling exercises. Most of the challenges they enountered were related to technical difficulties, to prior experiences with modelling, and to their attitude and focus.

The students encountered a couple of technical difficulties during the modelling activity. The challenges that they encountered as well as an explanation is highlighted in table 2 below.

Table 2: Technical difficulties students encountered during the modelling activity

Challenges	**Explanation**
The models were getting 'messed up' or producing an error	Even after numerous testing, some of the models were getting distorted or producing errors depending on the device being used by the students. Network connections were too slow.
Too much time and energy consumed opening the files	In order to save time and energy models were pre constructed for the students. All they needed to do was to drag the files to Edumol to open it. However, students still seemed to find it quite challenging; hence it took up quite a lot of their time and energy. This caused them to focus more on the satisfaction of opening the files rather than on visualizing and thinking about the model itself.
Unfamiliarity with Edumol	A few students pointed out that being unfamiliar with Edumol was a hindrance to their learning. They would have preferred to have been familiarized with it prior to doing the exercises.
Functionality of Edumol	A student mentioned that "Edumol program was a bit fiddly". Although, majority of the students seemed to have managed quite well with Edumol. Some students were finding it difficult due to the network conditions and the capability of their devices.
Language of Edumol	The language displayed on Edumol is dependent on the language of the device being used. Hence, even though some students desired to change the language of Edumol, they could not.
Too laborious to have to open so many models	One student mentioned that it was too laborious to have to open so many models.

Students prior experiences, or lack there of it with, modelling seemed to hinder their productivity with the computer-based molecular modelling. Some of the main points regarding the challenges they encountered are highlighted in table 3 below.

Table 3: Challenges caused by prior experience with modelling

Challenges	**Explanation**
Preference for physical models	Students had previously used physical models to model similar molecules. A few students expressed the desire to use physical models rather than computer-based ones. Students expressed that they "learn more when creating physical models".
Computer-based molecular models unnecessary to answer questions and explain bonding	A few students also expressed that the knowledge they acquired during class was sufficient to answer the questions and that they found that the molecular models didn't add much to their knowledge.
Unfamiliar method of learning	Some students mentioned that the entire activity was "so different to what we previously have done in class". Students expressed that they found the new learning method inhibiting, merely because it was new.

The rest of the challenges that the students seemed to have encountered while doing the exercises were due to certain attitudes towards the exercise and a lack of focus. If at all the greatest hindrance to their learning seemed to have been their attitudes and lack of focus. The student's opinions are highlighted in table 4 below

Table 4: Student attitudes that seemed to inhibit learning

Challenges	**Explanation**
Distaste for the use of electronic devices as learning tools	A couple of students expressed that they disliked using electronics as a learning tool. This clearly inhibiting their ability to learn. One student mentioned that they would have liked to use the computer-based models for work at home, "in class I'd like to make more use of the teachers expertise".
Exercise perceived as a test	Since students were asked to write down answers to the questions some viewed the entire experience as a test. This diverted their focus from learning and thinking to avoiding making mistakes.
Desire to avoid thinking	A few students preferred to look at their books for answers/information rather than focus on figuring it out by examining the models and thinking.
Decline in self confidence	A couple of students mentioned that "I realized how little I actually know, and it made me feel insecure about my knowledge". This seemed to have then inhibited their ability to effectively and productively focus on the task.
Lack of interest in visuals	A student mentioned that "I'm more of an auditory learner than visual".
Not challenging enough	A few students seemed to find the exercise "too easy"; hence claiming to have gained nothing from the modelling exercise.
Clear distinction between explanations and questions	A few students complained about the lack of a clear distinction between the explanation part and the questions on the exercise sheet. Additionally, a few students expressed concerns regarding the clarity of the first question.

Some of the Most Useful Features of Computer-based Molecular Modelling

Regardless of the challenges the students encountered while doing the exercises, they also seemed to have noticed a few features of Computer-based molecular modelling that seemed enhanced their understanding of bonding. The useful features mentioned by students are presented in table 5 below.

Table 5: Useful features of Computer-based molecular modelling

Feature	**Explanation**
3D visualization of molecules	Many students mentioned the importance/usefulness of being able to visualize the molecules three dimensionally. Some students really appreciated the value of it: "I'm a very visual learner, and this gave me visualizations to ideas that were pretty abstract in my mind before this".
Visualizing various bond types	Students also seemed pleased to be able to visualize the diverse types of bonding.
Visualizing hydrogen bonding as an example of intermolecular bonding	Many students seemed to appreciate the ability to view the hydrogen bonding in water, mentioning that it enhanced their understanding of hydrogen bonding.
Visualizing the molecular electrostatic potential (MEP)	Many students mentioned the advantages of being able to visualize the MEP. Mentioning how useful it was in visualizing partial charges as well as in noticing similarities between ionic and covalent bonding.
Measuring bond length	A few students mentioned that measuring the bond length was very useful.

Supporting Students Usage of Computer-based Molecular Modelling

In addition to the useful features of computer-based molecular modelling, students also mentioned a couple of general features of the exercise that supported them in using computer-based molecular modelling to understand/make sense of bonding. The aspects that seemed to have supported them are presented in table 6 below.

Table 6: Supporting students use of computer-based molecular models

Feature	Explanation
Short explanations together with the questions	Many students mentioned that the short explanations prior to the questions were very helpful.
The questions	Quite a few students mentioned that they liked “the way the questions guided my thought, such that I often did not feel completely on my own”. Additionally, “the idea of having a paper exercise sheet in conjunction with the computer software really synergized”.
Using models to understand concepts of chemistry	Some students valued being able to use models to make sense of concepts of chemistry. One student mentioned that it was useful “using the models for learning and understanding”.
Answering questions	While some students felt that answering the questions seemed more like a test and hence stressful. Others found answering the questions enjoyable and a learning experience.
The exercises focus on the fact that ionic and covalent bonding are not dichotomous	Many students appreciated the way the exercise led them to discover that ionic bonding and covalent bonding should not be viewed as a dichotomy but more as continuous pattern.
The exercises focus on shifts between macroscopic and molecular levels	Analysis of the concept maps indicated that after completing the modelling exercise students were more focused on making connections between the macroscopic and molecular levels. The concept maps also indicated students stronger focus on the physical properties of materials in relation to bonding, after doing the exercises.
Focus on electrostatic forces/attractions as an explanation for bonding rather than physiological needs/wants	The concepts maps created by the students after going through the exercise indicated an increase in the use of electrostatic forces/attractions as an explanation for bonding.

Quantitative results presenting students opinions

The questionnaire posed three closed-ended questions, in order to get an overview of student's opinions regarding the modelling exercises. Table 7 below presents the students opinions on whether they found the activity enjoyable. One the reasons this question was posed is because it is essential for students to enjoy activities in order to truly learn.

Table 7: Students opinions on whether they enjoyed the exercise

Answers	Yes	It was ok	No
Percentage (%)	39	46	15

Table 8 below presents the students opinions on whether they considered the visualization to have enhanced their understanding of bonding. Students provided various reasons for their answers which are highlighted in the tables above; however, table 8 provides an overview of their opinions.

Table 8: Students opinions on whether the visualizations enhanced their understanding of bonding

Answers	Yes	Sometimes	No
Percentage (%)	38	31	31

Table 9 below presents the students opinions on whether the questions were too difficult, perfect, or too easy. This was inquired in order to analyse the effectivity of the questions themselves.

Table 9: Students opinions on whether the exercise was easy, just right, or difficult

Answers	Easy	Just right	Difficult
Percentage (%)	15	54	31

6.3 Reliability of Results

The reliability of design research results can be confirmed through triangulation from multiple data sources (Design-Based Research, 2003). This research utilized concept mapping and questionnaires as data sources. The reliability of design research could also include an evaluation of it usefulness and improvements in teaching and learning (Design-Based Research Collective, 2003; Edelson, 2002). The design product (the exercise), provides useful information on the type of challenges students encounter when using computer-based molecular modelling to explain and understand chemical bonding. It also provides useful suggestion on how to support students use of computer-based molecular models. The design product could be used to teach and learn chemical bonding in high school chemistry.

Few ideas presented in the results chapter were gathered from the analysis of the concept maps, the reliability of those ideas could be questioned. Since students were quite unclear on the idea of creating concept maps and were more focussed on 'just adding something' However, majority of the research results are directly based on student's opinions expressed through the questionnaire or discussed during the research process. These results appear to be relatively reliable as students unwilling to express their opinions merely refrained from answering. Never the less a couple of complications with the research method were discovered during the research process. These complications could possibly have an effect on the reliability of the results. The problems encountered were that students found it difficult to create concept maps with the computer, student's prior experiences with similar models seemed to hinder the research, and students seemed to be quite overwhelmed.

For many students creating concept maps seemed to be a completely new and difficult experience. Even after they were explained about concept maps, briefed on how to create them and presented with examples of concept maps, they didn't seem to grasp the idea well. Many of the students mentioned that they disliked it as a means of presenting their knowledge. Additionally, requiring students to create concept maps on the computer seemed to add further confusion. The students hence became more focused on how to create a concept map on the computer than on the actual presentation of their knowledge. Many students expressed the need for more help and practice with creating the concept maps. Finally, students also mentioned that they felt the web based software used for creating the concept maps was not user friendly.

Having studied the topic previously with their teacher, seemed to hinder the research for a few reasons. Many of the student's main aim seemed to be getting a good score on their final exams; hence they viewed the research exercise as a "waste of time" rather than a learning experience. Additionally, having viewed similar models as physical models, was expressed to be slightly repetitive by students. It was also mentioned that a lot of the information was not new to them.

One of the major hindrances to the research was that most of the students seemed overwhelmed with the exercise. One main reason for this was that there were too many exercises for them to go through. This was because the exercise was designed to be used in parts; however, for research purposes it was used as a whole. Many of the students mentioned that having to do so many exercises was exhausting. Additionally, some students seemed to be slightly overwhelmed and insecure regarding their lack knowledge, hence hindering their concentration and understanding. Added to that, some students saw it as a test, which was another reason that they were overwhelmed. Furthermore, some students found it too challenging, while others felt they were “wasting too much class time on it”. A final factor that seemed to overwhelm them was the timing of the lesson (8am), many students claimed that “it was too early in the morning to think”.

6.4 Improvements Based on Research

This chapter discusses the improvements made based on the research results. First of all, the improvements made to the exercise are discussed. After which, suggestions for implementation during lessons are discussed. Then finally, possible improvements to the research method are discussed.

6.4.1 The Exercise and the Models

Students didn’t seem to face any difficulty understanding/utilizing the models. After analysing the research, it is evident that the models themselves were appropriate for the task and effective. However, students did experience technical difficulties when opening the models, an area that needs improvement. The research results suggested that the exercise sheet/instruction needed a few improvements. Students expressed the desire for a clear distinction between the questions and information. Additionally, a few students mentioned the need for the first questions to be more clearly stated. Taking the observations during the research and the students suggestions into consideration, the exercise sheet was redesigned (see appendix 3).

In addition to the changes made to the exercise sheet research also indicated a few ideas that need to be taken into consideration when utilizing computer-based molecular modelling (specially when utilizing it for the first time). These ideas are displayed in table 10 below. The ideas presented in table 10 are mainly suggestions related to the challenges that students encountered. However, when utilizing computer-based molecular modelling in a classroom situation teacher should also consider the useful features of computer-based molecular models and the supportive elements presented in tables 5 and 6.

Table 10: Suggestions for teachers utilizing computer-based molecular modelling in class

Suggestion	**Explanation**
Test devices earlier	Prior to the lesson student's devices should be tested to check if they can handle opening the models. However, if the school has a computer room with identical devices that are able to handle the models, using the computer room would be more logical.
Students could familiarize themselves with the computer-based molecular modelling software earlier	Students should familiarize themselves with computer-based modelling prior to actually doing the exercises, in order to ensure that the time spent doing the exercises is utilized to think about concepts of chemistry rather than the modelling software itself.
Utilize computer-based models when appropriate	Using models at the wrong time, such as, after having previously shown students an effective non-computer-based model, could give students the idea that computer-based models are unnecessary. This could possibly inhibit students from noticing the unique characteristics of computer-based modelling
Use both physical and computer-based models	Using both computer-based models as well as physical models could be highly effective. First of all, students who prefer physical models will benefit. Secondly, the additional features of computer-based modelling will be utilized productively. And finally it could be the perfect opportunity to provide students with a variety of models, allowing them to analyse the limitations of models.
Promote the idea of learning	Try to promote the idea that the exercise is not a method of testing how much students know but a method of supporting learning.
Provide more challenging tasks for students who need it	Naturally some students might find the tasks easier then others (as indicated in table 9). In that case, be prepared to provide them with more challenging tasks to keep them interested and in order to enhance their learning process.
Practice making concept maps	If teachers desire students to display their understanding of bonding through a concept map. It is importance to introduce concept mapping in advance and to encourage them to practice

6.4.2 Implementation during a lesson

Carrying out the research in a classroom environment, suggestions from the students and discussions with their teacher brought up various other possible methods of implementing computer-based molecular exercises during a lesson. These ideas are highlighted in this chapter.

As a Demonstration

Rather than asking students to open the computer-based models individually, the teacher could display them on the board for the students to observe. Opening the models could be more of a teacher centred task than a student centred one. It would save a lot of time and eliminate the challenges students encountered due to their devices. This could possibly encourage students to focus on the models rather than on the modelling software.

Discussions rather than answering questions on paper

The exercise could also be done in groups of 3-4. Students could be asked to examine the models and discuss the answers to the questions groups. This way, students might not feel like the exercise is a test and they might enjoy it more. Also discussing the models and concepts of bonding could enhance student understanding of bonding.

Homework tasks

The exercise could also be given to the students as homework tasks. A few students seemed to have liked the idea of utilizing the computer-based software to assist them at home with visualizations.

6.4.3 Improvements to the research method

Having carried out the first phase of the research, and having modified the exercise sheet, if the research were to be conducted again, it would be necessary to take the ideas presented below into consideration.

Concept maps

If concept maps are being used for students to display their knowledge, it is of high importance that students are introduced to the idea of making concept maps and that they practice creating concept maps prior to taking part in the research. Additionally, if the concept maps are being created on the computer, it must be confirmed with the students that they are comfortable with using computers to create concept maps. If they aren't, the possibility of using pen and paper should be considered. Because it seemed like using the computer to create concept maps significantly inhibited student's ability to display and reflect on their knowledge.

Prior experiences

If the topic has previously been covered by the teacher, the students might find the task repetitive, thus inhibiting learning. The research could also be conducted in sync with the teacher's lectures. Students could carry out the tasks as the teacher covers each topic, since the tasks are essentially designed to be used this way in the classroom. This method could avoid the problem of students feeling that the information is repetitive. Furthermore, students might not feel too overwhelmed and they might not resent 'wasting too much time' for the research.

Avoid overwhelming situations

One could also attempt to avoid situations in which students feel overwhelmed while doing the exercises. The timing of the research is one aspect that could be considered, it might be easier on the students if the research is carried out at around 9 am rather than 8 am. Additionally, the idea of learning must be promoted, in order to avoid students from focusing on how much they don't know.

7. Conclusion and Discussion

This chapter presents the conclusions and discussions of this thesis. The first subchapter discusses the challenges that students encountered when using computer-based molecular modelling. After which, the second sub chapter discusses supporting students with the use of computer-based molecular modelling. Then finally, the third sub chapter discusses implications of this research.

7.1 Challenges Students encountered when using Computer-based Molecular Modelling

Conclusively, students encountered various challenges when using computer-based molecular models to enhance their understanding of bonding, specially since they were using computer-based molecular models for the first time. The challenges were generally related to technical difficulties, students prior experience with models and their attitude.

Research showed that there were a few significant challenges that students encountered due to technical difficulties. As Aksela and Lundell (2008) point out, schools need to posses the proper equipment. The research results of this study also strongly suggest the need for proper equipment that is capable of handling the models. Based on the research results it was also evident that too much time and energy should not be consumed on opening models. It has a negative effect on students learning because students focus more on opening the models rather than focusing on understanding the models. Furthermore, it is possible to conclude that familiarizing students with computer-based molecular modelling prior to using it as a tool for explaining chemistry is necessary. It will allow students to focus on understanding and explaining rather than learning the functionality of the program. Finally, the research indicated that it is essential for students to be able to easily change the language of the modelling program in order to work productively.

Students prior experiences with modelling could also indirectly be the root of some of the challenges students encounter. The research results suggest that having used physical models prior to computer-based models, students might prefer using physical models. Hence, it is important to convey the unique functions of computer-based modelling to students. Previous research (Aksela & Lundell, 2008) also suggests using physical models in conjunction with computer-based models. Furthermore, the research results also suggested that if a method of learning is unfamiliar to students, it could inhibit their learning. Garvin (1991) confirmed that students are uncomfortable with new approaches to learning. Hence, using models to understand and explain chemical concepts could briefly be introduced to students in the form of examples during lectures, to ensure that students don't feel overwhelmed by an unfamiliar method of learning.

The research results indicate that student's attitudes are significant when using computer-based models to enhance understanding of bonding. During the designed activity students encountered a couple of challenges due to their attitudes. Some students seemed to dislike using electronics as learning devices. Therefore, it is essential that teachers highlight the unique uses of computer-based models in order to illustrate their importance. Additionally, the research results indicate that teachers must emphasize that the focus of using models to explain/understand chemical concepts is to learn. Students perceiving the exercise as a test inhibited their ability to learn. Perceiving the modelling exercise as a test, resulted in students loosing self confidence and their loss in self confidence then further inhibited their ability to learn. Research also indicated that teachers should direct students to reflect on the models and on the concepts of bonding, in order to use computer-based models efficiently to explain and understand bonding. Many students preferred, to check their books for answers rather than to think and reflect themselves. Furthermore, research (Gunter et al., 1993) suggests that a mismatch between student ability and task difficulty could be problematic. Likewise, the research results of this study indicate that teachers must provide activities that are challenging enough for students.

7.2 Supporting Students learning with the use of Computer-based Molecular Modelling

In order to support students understanding of bonding with the use of computer-based molecular modelling, it is necessary to know what features of computer-based modelling enhance student understanding and how to support students use of computer-based molecular modelling. The research results highlighted a couple of useful features of computer-based molecular modelling that enhance student understanding of bonding, based on student's

opinions. The research results also suggest how to support students use of computer-based molecular models in order to enhance understanding of bonding.
The results of this study provided a list of a few features of computer-based models that students found useful in enhancing their understanding of bonding (table 5). Previous researches (Hehre & Shusterman, 2000; Shusterman & Shusterman, 1997) have also presented the usefulness of the features mentioned. Students found the 3D visualization of molecules to be highly productive in illustrating the abstract concepts of bonding. They also appreciated the possibility of visualizing various types of bonding (ionic, covalent, metallic), mentioning that it enhanced their understanding of bonding. The value of being able to visualize hydrogen bonds as an example of intermolecular bonding was also mentioned. Additionally, students conveyed that visualizing the molecular electrostatic potential (MEP), enhanced their understanding of partial charges as well as their understanding of polar covalent compounds. Finally, it was also indicated that being able to measure the bond length in order to investigate correlations between bond length and bond order was beneficial.

The research results also provided a couple of ideas to consider/use when using computer-based modelling to enhance students understanding of bonding. Providing short explanations to the theory of bonding together with questions to be answered with the help of computer-based models, proved to be useful. Students found that it guided their thoughts and prevented them from feeling lost. Using the models for learning and understanding concepts of chemistry appeared to be favourable among some students. However, having to answer questions in written form proved to be an efficient learning experience for some, and a stressful test-like experience for others. Hence it is important to understand if students prefer to answer question in written form or discuss the questions with their peers, in order to ensure a productive learning experiences for students. Teachers can/should individualize the activity based on student preferences.

The research results also indicated that using computer-based molecular models to explain concepts of bonding, enhanced student's ability to successfully shift between macroscopic and molecular levels. It also enhanced the student's ability to focus on electrical forces/attractions as an explanation for bonding rather than physiological needs/wants. The mentioned results have also been confirmed by previous researches (Frailich, Kesner & Hofstein, 2009).

7.3 Implications of the Research

As mentioned in chapter 4, modelling is an essential tool to understand chemistry since few of the macroscopic observations can be understood without the assistance of sub-microscopic representations of models (Oversby, 2000). Computer based molecular modelling has opened various possibilities for teaching as computer-based molecular models possess various features that further assist in using sub-microscopic representations of models to understand macroscopic properties. (Aksela & Lundell, 2008; Hehre & Shusterman, 2000)

Since the importance and potential of computer-based molecular modelling has already been highlighted through the results of previous researches, the aim of this research was to focus on **how** to use computer-based molecular modelling to enhance student understanding of bonding. The research focused on student's thoughts, opinions and feelings. The results strongly imply the need for well planned exercises in order to effectively use computer-based models to enhance students understanding of bonding.

Prior to the lesson teachers must minimize the risks of technical difficulties, as frustrations with technical difficulties could render the activity practically useless. Teachers must consider the particular needs of the students and avoid situations in which students might feel overwhelmed by tasks. Ignoring students needs, and allowing them to feel overwhelmed could create negative feelings towards the task inhibiting student from productively learning. Teachers must also focus on using the features/functions of computer-based models that are known to be highly effective in enhancing the understanding of bonding. By focusing on such features the teacher could ensure that students understand the value/importance of computer-based models thus promoting positive attitudes. Additionally, focusing on using the most effective features will enhance student's understanding of bonding. Furthermore, teachers should aim to provide as much support and guidance to students as possible. Teachers could use brief written explanations and questions to guide student's thoughts. The guidance should aim to encourage students to focus on important aspects of bonding and to eliminate alternative conceptions. It is important for teachers to individualize the modelling activity for students, in order to ensure productive learning.

Based on the research conducted improvements were made to the original design of the exercise. Further research is necessary to analyse whether the improvements to the original design make a significant difference. Table 8 illustrates the opinions of students regarding whether they considered the visualizations to have enhanced their understanding of bonding. 38% of the students thought it did, 31% thought it did sometimes and 31% thought it did not enhance their understanding of bonding. Since these statistics are based solely on student opinions it would be useful to further research the extent to which computer-based molecular modelling enhances student understanding of bonding. The research could be conducted by utilizing concept maps more effectively, to acquire a deeper insight on students understanding of bonding. Further research could also be conducted to produce an ideal method to introduce computer-based molecular modelling to students, aiming to ensure that students learn to use it efficiently to understand and explain chemical concepts.

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Appendices

Appendix 1: Initial Exercise design

Ionic bonds

In Edumol open (on different tabs): 1. NaCl, 2. Saltcrystal, and 3. Water

Visualize the saltcrystal as a CPK model as well

1. Sodium Chloride is a classic example of an ionic bond. During the formation of sodium chloride, energy is required for the following steps: 1. Cl-Cl bond is broken, 2. $Na_{(s)}$ to $Na_{(g)}$, and 3. Ionization of $Na_{(g)}$ to Na^+. Energy is released when $Cl_{(g)}$ gains an electron (Cl^-). Yet the formation of NaCl from Na and Cl_2 is an exothermic reaction. Explain based on electrical forces, why it is an exothermic reaction.

2. Ionic compounds have distinct properties:

a) Aqueous solutions of ionic compounds conduct electricity.

b) Ionic compounds are soluble in polar solvents. For example, sodium chloride is soluble in water (polar solvent).

Draw your own model of what an aqueous solution of NaCl looks like based on the models of water and salt. Explain your model, also explain why aqueous solutions of ionic compounds conduct electricity.

c) Ionic crystals are relatively hard but quite often brittle (break easily). Use the above viewed salt CPK model to explain why ionic crystals are brittle. (Hint: think what happens to the ions if you hit a crystal of salt with a knife or spoon)

d) The melting and boiling points of ionic compounds are usually very high (Sodium chlorides melting point is 801° and its boiling point is 1413°C). Can you explain this based on the structure of ionic compounds.

e) The Volatility of ionic compounds tends to be very low. Can you explain this? (volatility: the tendency of a substance to vaporize).

Covalent bonds

Simple Covalent compounds

3. In a covalent bond electrons are shared between atoms. Cl_2 and HCl are both bonded covalently. Open in Edumol (on different tabs) the files HCl and Cl2, visualize the MEP. Explain the electron distribution of Cl_2 and HCl based on the visualization. Also explain why HCl is a polar covalent compound and Cl_2 is a covalent compound.

Covalent bonds between atoms ***within*** a molecule are very strong. The forces of attraction ***between*** the molecules are generally much weaker. These intermolecular forces depend on the polarity of molecules. Polar molecules are held together mainly by **dipole-dipole** intermolecular forces between molecules and non-polar molecules are held together mainly by **Van der Waals forces (dispersion)** between molecules.

Dipole-dipole forces (intermolecular forces)

4. Polar covalent bonds, result in polar molecules (molecules with permanent dipole moments δ^+ and δ^-). Open the file ICl in Edumol and visualize the MEP. Based on your visualization draw the **intermolecular forces** between three ICl molecules and explain the electrostatic attractions.

5. **Hydrogen bonding** is a stronger dipole-dipole attraction, it occurs when hydrogen is bonded directly to a small highly electronegative atom such as fluorine, oxygen or nitrogen. As the electron pair is drawn away from the hydrogen atom by the more electronegative atom, all that remains is the proton in the nucleus since there are no inner electrons. The proton then attracts a pair of non-bonding electrons from the F, O or N.
Open the file water in Edumol and visualize the hydrogen bonds.
Open the file ice in Edumol and visualize the hydrogen bonds.

6. What factors affect the strength of dipole-dipole bonding?

Van der Waals Forces (intermolecular forces)

Even in non-polar covalent molecules (such as He) the electrons can be unevenly spread at any moment, producing temporary (instantaneous) dipoles. An instantaneous dipole can induce another dipole in neighbouring particles resulting in weak attractions between two particles, such as seen in figure 1 below.

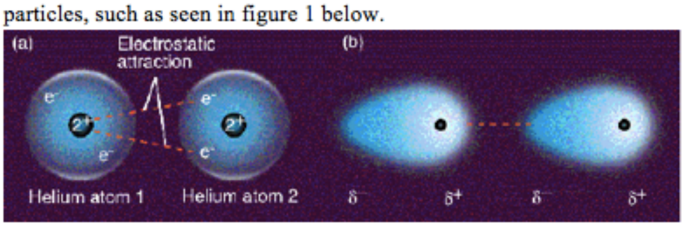


Figure 1: Induced dipole of a helium atom (Oakland Schools Chemistry Resource unit)

7. Explain why Van der Waals forces increase with increasing mass.

8. Simple covalent compounds have distinct properties. Explain the following based on the electrostatic attractions

a) Covalent compounds have low melting and boiling points and high volatility

b) In their solid, liquid and gas states covalent compounds do not conduct electricity. Similarly, in solutions they do not conduct electricity.

c) Explain the solubility of the following covalent compounds: ethane and ethanol. Also discuss the solubility of heptanol. You can visualize the structure as well as the MEP to guide you if necessary. Open in Edumol Q8

Giant covalent compounds

9. Giant Covalent structures contain numerous atoms joined to adjacent atoms by covalent bonds. The atoms are usually arranged in giant regular lattices. Diamond and graphite and are giant covalent structures. Open in Edumol Diamond and Graphite(e) to visualize the structure of Diamond and graphite. Notice the delocalized electrons between the layers of graphite.

a. Explain based on the model why graphite is soft and slippery, has a high melting point and conducts electricity.

b. Explain based on the model why diamond is hard, has a very high melting point (more than 3600°C) and does not conduct electricity

Metallic bonding

10. Metals form giant structures in which valence electrons of the metal are free to move. When valence electrons in metals become detached from the individual atoms, metals consist of positive ions and delocalized electrons. Open in edumol the file gold to view the structure of gold as an example of metallic bonding. Explain metallic bonding by the electrostatic attractions

11. Most metals have distinct properties (although, the extent of their properties differs depending on the metal, for example some are better conductors of electricity then others). Explain the following based on the structure of metals:

a) Metals are malleable and ductile

b) Metals have high melting and boiling points

c) Metals conduct electricity

Similarities between, ionic, covalent and polar covalent bonding

12. Open in Edumol the file NaCl, Cl2 and HCl, visualize the MEP
Generally, it is possible to predict if a compound has ionic or covalent bonds based on the difference in electronegativity. If the difference in electronegativity between atoms is greater than 1,8 than it is usually ionic. However, often compounds are somewhere in between ionic and covalent. In reality these bonding types are merely modifications of the same basic pattern. Based on your knowledge of ionic, polar covalent and covalent bonds and the models explain why ionic and covalent bonding should **not** be viewed as a dichotomy?

Bond length

Bond length is the average distance between the centres of the nuclei of two bonded atoms in a molecule. The shorter the bond length is, the larger the bond energy. It is measured in Angstrom units (Å) or picometers (pm).

13. What is the relation between the bond length and the size of the bonded atoms? Examine the bond length of F_2, Cl_2, and Br_2 to assist you in your explanation.
Open in Edumol the file Q13

14. What is the relation between bond length and bond order (number of chemical bonds between a pair of atoms)? Examine the bond lengths between the carbon atoms of ethane, ethene and ethyne to assist you in your explanation.
Open in Edumol the file Q14

Appendix 2: Questionnaire

Questionnaire

1. Did you enjoy the exercise? (please give a reason for your answer)

2. Was the exercise too easy, too hard, or just right?

3. Did the visualization of the models enhance your understanding of chemical bonding? (please give a reason for your answer)

4. What did you like most about the exercise? Why?

5. What aspects of the exercise helped you learn/understand? Explain your answer.

6. Would this be a useful class activity while studying the topic?

7. Is there anything you would change in the exercise? Why?

Appendix 3: Redesigned Exercise

Ionic bonds

In Edumol open (on different tabs): 1. NaCl, 2. Saltcrystal, and 3. Water

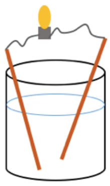
Visualize the saltcrystal as a CPK model as well

Sodium Chloride is a classic example of an ionic bond. During the formation of sodium chloride, energy is required when: 1. Cl-Cl bond is broken, 2. Sodium changes state from solid to gas and 3. Gaseous sodium is ionized. Energy is released when gaseous chlorine gains an electron. Yet the formation of NaCl from Na and Cl_2 is an exothermic reaction.

Question 1: Explain based on electrical forces, why the formation of sodium chloride is an exothermic reaction.

Ionic compounds have distinct properties:

a) Aqueous solutions of ionic compounds conduct electricity.



b) Ionic compounds are soluble in polar solvents. For example, sodium chloride is soluble in water (polar solvent).

c) Ionic crystals are relatively hard but quite often brittle (break easily).

d) The melting and boiling points of ionic compounds are usually very high (Sodium chlorides melting point is 801° and its boiling point is 1413°C).

e) The Volatility of ionic compounds tends to be very low (volatility: the tendency of a substance to vaporize).

Question 2:

a & b) Draw your own model of what an aqueous solution of NaCl looks like based on the models of water and salt. Explain your model, also explain why aqueous solutions of ionic compounds conduct electricity.

c) Use the above viewed salt CPK model to explain why ionic crystals are brittle. (Hint: think what happens to the ions if you hit a crystal of salt with a knife or spoon)

d) Can you explain property d based on the structure of ionic compounds.

e) Can you explain property e?

Covalent bonds

Simple Covalent compounds

In a covalent bond electrons are shared between atoms. Cl_2 and HCl are both bonded covalently. Open in Edumol (on different tabs) the files HCl and Cl2, visualize the MEP.

Question 3: Explain the electron distribution of Cl_2 and HCl based on the visualization. Also explain why HCl is a polar covalent compound and Cl_2 is a covalent compound.

Covalent bonds between atoms ***within*** a molecule are very strong. The forces of attraction ***between*** the molecules are generally much weaker. These intermolecular forces depend on the polarity of molecules. Polar molecules are held together mainly by **dipole-dipole** intermolecular forces between molecules and non-polar molecules are held together mainly by **Van der Waals forces (dispersion)** between molecules.

Dipole-dipole forces (intermolecular forces)

Polar covalent bonds, result in polar molecules (molecules with permanent dipole moments δ^+ and δ^-). Open the file ICl in Edumol and visualize the MEP.

Question 4: Based the visualization draw the **intermolecular forces** between three ICl molecules and explain the electrostatic attractions.

Hydrogen bonding is a stronger dipole-dipole attraction, it occurs when hydrogen is bonded directly to a small highly electronegative atom such as fluorine, oxygen or nitrogen. As the electron pair is drawn away from the hydrogen atom by the more electronegative atom, all that remains is the proton in the nucleus since there are no inner electrons. The proton then attracts a pair of non-bonding electrons from the F, O or N.

Open the file water in Edumol and visualize the hydrogen bonds.

Open the file ice in Edumol and visualize the hydrogen bonds.

Question 5: What factors affect the strength of dipole-dipole bonding?

<u>Van der Waals Forces (intermolecular forces)</u>

Even in non-polar covalent molecules (such as He) the electrons can be unevenly spread at any moment, producing temporary (instantaneous) dipoles. An instantaneous dipole can induce another dipole in neighbouring particles resulting in weak attractions between two particles, such as seen in figure 1 below.

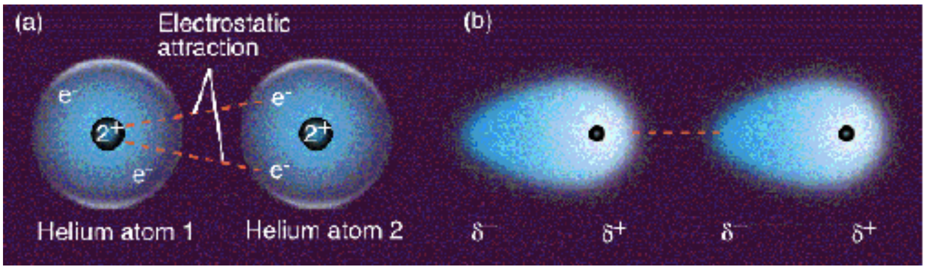


Figure 1: Induced dipole of a helium atom (Oakland Schools Chemistry Resource unit)

Question 6: Explain why Van der Waals forces increase with increasing mass.

Question 7: Simple covalent compounds have distinct properties. Explain the following based on electrostatic attractions

a) Covalent compounds have low melting and boiling points and high volatility

b) In their solid, liquid and gas states covalent compounds do not conduct electricity. Similarly, in solutions they do not conduct electricity.

c) Explain the solubility of the following covalent compounds: ethane and ethanol. Also discuss the solubility of heptanol. You can visualize the structure as well as the MEP to guide you if necessary. Open in Edumol Q7

Giant covalent compounds

Giant Covalent structures contain numerous atoms joined to adjacent atoms by covalent bonds. The atoms are usually arranged in giant regular lattices. Diamond and graphite and are giant covalent structures. Open in Edumol Diamond and Graphite(e) to visualize the structure of Diamond and graphite. Notice the delocalized electrons between the layers of graphite.

Question 8: Explain based on the model why graphite is soft and slippery, has a high melting point and conducts electricity.

Question 9: Explain based on the model why diamond is hard, has a very high melting point (more than 3600°C) and does not conduct electricity.

Metallic bonding

Metals form giant structures in which valence electrons of the metal are free to move. When valence electrons in metals become detached from the individual atoms, metals consist of positive ions and delocalized electrons. Open in edumol the file gold to view the structure of gold as an example of metallic bonding.

Question 10: Explain metallic bonding by the electrostatic attractions

Most metals have distinct properties (although, the extent of their properties differs depending on the metal, for example some are better conductors of electricity then others).

Question 11: Explain the following based on the structure of metals:

a) Metals are malleable and ductile

b) Metals have high melting and boiling points

c) Metals conduct electricity

Similarities between, ionic, covalent and polar covalent bonding

Open in Edumol the file NaCl, Cl2 and HCl, visualize the MEP

Generally, it is possible to predict if a compound has ionic or covalent bonds based on the difference in electronegativity. If the difference in electronegativity between atoms is greater than 1,8 than it is usually ionic. However, often compounds are somewhere in between ionic and covalent. In reality these bonding types are merely modifications of the same basic pattern.

Question 12: Based on your knowledge of ionic, polar covalent and covalent bonds and the models explain why ionic and covalent bonding should **not** be viewed as a dichotomy?

Bond length

Bond length is the average distance between the centres of the nuclei of two bonded atoms in a molecule. The shorter the bond length is, the larger the bond energy. It is measured in Angstrom units (Å) or picometers (pm).

13. What is the relation between the bond length and the size of the bonded atoms? Examine the bond length of F_2, Cl_2, and Br_2 to assist you in your explanation.

Open in Edumol the file Q13

14. What is the relation between bond length and bond order (number of chemical bonds between a pair of atoms)? Examine the bond lengths between the carbon atoms of ethane, ethene and ethyne to assist you in your explanation.

Open in Edumol the file Q14

Appendix 4: Edumol files to be used in conjunction with the Exercise

The following link will provide access to the files that needed were opened in Edumol in conjunction with the exercise

https://drive.google.com/folderview?id=0B7GVjyey1_i9Rk1SczNQamZybEU&usp=sharing