THE ROLE OF MENTAL-MODELING ABILITY, CONTENT KNOWLEDGE, AND MENTAL MODELS IN GENERAL CHEMISTRY STUDENTS' UNDERSTANDING ABOUT MOLECULAR POLARITY

A Dissertation

presented to

the Faculty of the Graduate School

University of Missouri – Columbia

In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

by

CHIA-YU WANG

Dr. Lloyd H. Barrow, Dissertation Supervisor

AUGUST 2007

The undersigned, appointed by the Dean of the Graduate School,
have examined the dissertation entitled.

THE ROLE OF MENTAL-MODELING ABILITY, CONTENT KNOWLEDGE, AND MENTAL MODELS IN GENERAL CHEMISTRY STUDENTS' UNDERSTANDING ABOUT MOLECULAR POLARITY

Presented by Chia-Yu Wang

A candidate for the degree of Doctor of Philosophy.

And hereby certify that in their opinion it is worthy to acceptance.

Lloyd H. Barrow

Dr. Lloyd H. Barrow, Dissertation Supervisor

Sandra K. Abell

Dr. Sandra K. Abell

Mark J. Volkmann

Dr. Mark J. Volkmann

David J. Robertson

Dr. David J. Robertson

Mark Ehlert

Dr. Mark Ehlert

ACKNOWLEDGEMENTS

I first want to extend my deepest gratitude to my doctoral advisor, Dr. Lloyd Barrow, who set no limit allowing me to explore freely in science education research. I can't thank you enough for your guidance and endless support throughout my entire doctoral program. You always stood by me and had faith in me. You have allowed me to grow at my own pace.

I would also like to acknowledge my other committee members: Dr. Sandra Abell, Dr. Mark Volkmann, Dr. Mark Ehlert, and Dr. David Robertson. It is very difficult to express my thanks in a limited paragraph because each of you has contributed greatly to my knowledge and research ability of science education from different perspectives. What you have taught me is far beyond this dissertation work. Thank you Dr. Abell and Dr. Volkmann for being great models of mentors and researchers. Your friendship will always have a special place in my heart. Thank you Dr. Ehlert – my experience working with you on the professional development project has prepared me to have a critical eye to examine quantitative data and a sensitive mind to explore the dynamic interactions in an educational setting. Dr. Robertson, thank you for opening your class and offering your support throughout my study. The experiences of being a student and a researcher in your courses opened a window for me into the dynamic interactions of undergraduate chemistry classrooms.

I also want to thank my science education colleagues for their friendship and all the joyful times that we have shared. Although I am not naming each of you, thank you for being there for me during my down times and cheering me up with your support and smiles. Pursuing my doctoral degree has become the greatest adventure of my life. Because of your company, this adventure has been full of joy and memories.

I express my special appreciation to Catherine Wissehr, Meredith Park Rogers, Patrick Brown, Kusalin Musikul, Kristen Hutchins, and Hung Chiao. Thank you for editing my work and providing your insight at the various stages of my study.

I also want to thank all of the participants in my study. Thank you for devoting your time and granting access to your information. Your participation was valuable to my study.

Last, but not least, I want to thank my parents, Hsun-Chiu Shih and Hsun-Ming Wang, for supporting me in pursuing my dream. Hui-Yu, my sister, thank you for being the best friend I could ever have. You are the first person I want to share the great news with: Here I am, holding my degree.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

THE ROLE OF MENTAL-MODELING ABILITY, CONTENT KNOWLEDGE, AND MENTAL MODELS IN GENERAL CHEMISTRY STUDENTS' UNDERSTANDING ABOUT MOLECULAR POLARITY

Chia-Yu Wang

Dr. Lloyd H. Barrow, Dissertation Supervisor

ABSTRACT

This study explored general chemistry students' thinking processes about molecular polarity and related concepts. The study employed a mixed-method design to reveal how general chemistry students use their conceptual frameworks and mental models to solve problems about molecular polarity. In the quantitative phase, I collected student background information (gender, the number of previous chemistry courses) and scores of course exams. Also, three diagnostic instruments were used to gather information in terms of students' understanding and misconceptions about concepts of molecular geometry, polarity, and prerequisite concepts. The design and implementation of the qualitative phase was guided by a theoretical framework of personal constructivism and a case study methodology. The primary data sources were video-taped interviews using a combination of think-aloud protocol and interview-about-events to elicit students' explanations and thinking processes. The secondary data sources were students' artifacts constructed during the interviews and their responses to the items on the three diagnostic instruments. Grounded theory approach, employing a constant comparative method, was used for data analysis.

The quantitative phase involved 159 students. The results of one-way ANOVAS indicated that there were no statistically significant differences for mean scores between male and female students on scores for Chemical Bonding (CB) Instrument (Jang, 2003; Peterson, Treagust, & Garnett, 1989), Geometry and Polarity (GP) Instrument (Furió, Calatayud, Bárcenas, & Padilla, 2000; Peterson et al., 1989), exams, or course grade. Only on Electronegativity (EN) Instrument (Taber, 2002b) were scores of male students significantly higher than scores of female students. Also, the results of one-way ANOVA showed that the effect of the number of previous chemistry courses was not statistically significant for students' scores on instruments EN, CB, and GP, four course exams, or course grade. Misconceptions associated with concepts of electronegativity, chemical bonding, bond polarity, molecular shape, polarity of molecules, intermolecular force, and ionic lattices are reported.

For findings from the qualitative phase, I characterized high-, moderate-, and low-scoring students' mental-modeling ability, conceptual frameworks, and features of mental models while solving problems about molecular geometry and polarity. The major finding is that there is a positive interdependent relationship between an individual's level of content knowledge and mental-modeling ability, where one may facilitate or hinder the other.

Findings on comparisons of each student's conceptual framework indicated three prerequisite concepts that may explain students' failure to learn about molecular geometry and polarity. The analyses of students' conceptual frameworks confirmed that when studying student learning about an advanced concept, the scope of the research needs to go beyond examining student understanding about a single concept. Instead, the study needs to incorporate prerequisite concepts to explore students' conceptual frameworks. I also found that metacognitive ability played a significant role in successful mental-modeling process. However, metacognition has not been discussed in research on students' mental models or model-based reasoning.

This study provided empirical evidence for how students' content knowledge, mental-modeling ability, and construction and use of mental models influence their understanding about molecular polarity. The findings have implications for college chemistry education of molecular polarity.

CHAPTER ONE

INTRODUCTION

Extensive research has been devoted to determine why chemistry concepts are difficult for students to understand. Science education researchers have identified various factors that may explain three learning impediments. These include: incorrect, low quality, missing or fragmented content knowledge (Krajcik, 1991; Taber, 2001a); learners' limited mental working space (Johnstone, 1991; Taber, 2001a), a low visuospatial thinking ability (Bodner & Domin, 2000; Briggs, 2004; Wu & Shah, 2004), insufficient understanding for the role of models (Taber, 2002a), and students' common sense reasoning (Furió & Calatayud, 1996; Furió et al., 2000; Talanquer, 2006).

According to Johnstone (1991; 1993), a new approach for learning and teaching chemistry needs to include three basic domains: (1) macrochemistry, where chemistry is experienced at the tangible, visible, and sensory level, (2) submicrochemistry, which explains macro-phenomena at the atomic and molecular level with the kinetic perspective, and (3) representational chemistry which includes symbols, equations, stoichiometry, and mathematics. These three domains of chemistry were represented as a triangle of chemical understanding (Figure 1). Chemistry experts are able to slide from one domain to another easily; however, students often encounter difficulties when transitioning from one domain to another. Literature about how students make transitions within Johnstone's triangle is limited and extensively focused on the transition from macroscopic to submicroscopic levels. Research on transitions between submicroscopic-symbolic and symbolic-macroscopic domains has been overlooked.

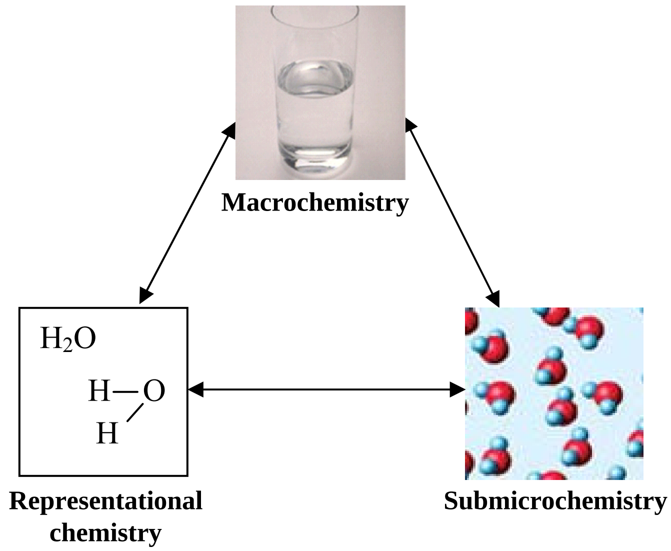


Figure 1. The triangle of chemical understanding (modified from Johnstone, 1993).

Learners experience everyday phenomena with their senses, but chemical concepts are usually explained at the symbolic level in the classroom. Teachers often assume that students are able to connect symbolic representations to submicroscopic models on their own. During the learning process, students' misunderstanding of the symbols are often neglected (Gabel, 1998). Research on students' ideas at the submicroscopic-symbolic domain often attributes students' misconceptions to two impediments: (1) the unfamiliarity with symbolic language and its level of abstraction (Marais & Jordaan, 2000) and (2) commonsense reasoning (Furió & Calatayud, 1996; Furió et al., 2000; Talanquer, 2006). Current research on problem-solving also found that students' ability to shift among chemical representations plays a critical role in their learning of chemistry (Bodner & Domin, 2000).

Molecular polarity is:

> A physical property of a substance which relates other physical properties such as melting and boiling points, solubility, and intermolecular interactions between molecules. It determines the strength and types of intermolecular forces in a sample of the substance. Molecular polarity

> results from the uneven partial charge distribution between or among various atoms in a molecule. This imbalanced charge can be observed when the molecules are placed in an electric field. (Ophardt, 2003, p. 1)

According to Chang (2005, p. 396), "the polarity of the whole molecule can be inferred from the magnitude of its dipole moment which is a vector joining the centre of positive charge to the centre of negative charge." Both bond polarity and molecular geometry need to be taken into consideration when determining whether a molecule is polar or nonpolar and its magnitude of polarity.

The concept of molecular polarity is usually introduced at the middle of a sequence of general college chemistry courses. Molecular polarity is built on concepts of atomic structure, periodic variation in the Periodic Table, chemical bonding, electronegativity, construction of Lewis structures, molecular geometry, dipole moment, and valance bond theory. It is also a prerequisite for learning more advanced concepts including intermolecular forces, properties of solutions, acids and bases, and organic chemistry.

Purpose of the Study and the Overarching Research Question

The purpose of the study was to investigate student thinking processes while solving problems about molecular polarity. Learning about molecular polarity requires an understanding of prerequisite concepts including electronegativity, bonding, molecular geometry, and dipole moment. Also, it requires thinking with symbols and models and visualizing spatial structure of a molecule in three dimensions (3D). Thus, it is a difficult concept for students to understand; yet research on this topic is limited to identifying chemistry students' common misconceptions about molecular polarity and its prerequisite concepts (Jang, 2003; Nicoll, 2003; Peterson & Treagust, 1989; Peterson et al., 1989). Only Furió and colleagues (1996; 2000) attributed one learning impediment to students' common sense reasoning. More research is needed to identify learning impediments that hinder students' learning about molecular polarity. It was this need that guided this study to investigate students' thinking processes on this abstract concept.

New research evidence showed that ability to construct and use mental models may affect students' conceptualization about chemical concepts (Bodner & Domin, 2000; Briggs & Bodner, 2005; Ferk, Vrtacnik, Blejec, & Gril, 2003; Stieff, Bateman, & Uttal, 2005). This study incorporated this new aspect to study general chemistry students' thinking processes about molecular polarity and related concepts. The overarching research question was: What are the influences on students' problem-solving about molecular polarity? By employing a mixed-method design, this study revealed relationships among students' fundamental knowledge and thinking with mental models and how these two aspects influenced students' learning about molecular polarity.

Conceptual Framework

Two areas of research guided the design, interpretation, and analysis of the study: fundamental knowledge and mental model. In the following subsections, these aspects are reviewed in relation to the context of this study.

Fundamental Knowledge

The first important conceptual framework that underlies this study is about human knowledge and how people use it to learn. Conceptual change theories (Chi, 1992; Chi, Slotta, & de Leeuw, 1994; Hewson, 1981, 1996; Hewson & Hewson, 1992; Mortimer, 1995; Posner, Strike, Hewson, & Gertzog, 1982; She, 2004; Strike & Posner, 1992; Vosniadou, 1994, 2003; Vosniadou & Ioannides, 1998) share a common view that human knowledge is schema-like, consisting of various interrelated conceptual components. The base of knowledge that one possesses about a specific concept varies among individuals due to their different prior knowledge and experience. Learners systematically and consistently conceptualize a new idea by applying this base of knowledge to assimilate it into the existing knowledge base. When this new conception is in conflict with their existing knowledge, the learners must reconstruct their prior knowledge to reconcile this new information. This prior knowledge also allows the learner to recognize a problem and to select appropriate existing conceptions for reasoning (Chi, 1992).

Posner et al. (1982) used 'conceptual ecology' to describe the general background knowledge which includes an individual's epistemological commitments to some subject-specific views, analogies, metaphors, metaphysical beliefs, and knowledge from different areas. This study included models and mental models as a part of the knowledge base. Research by Vosniadou and Ioannides (1998) has shown that an individual generates models and/or mental models based upon their knowledge base so they can assimilate or reconcile new information. These generated mental models are applied and tested in new situations (Eilam, 2004; Vosniadou & Brewer, 1992) and retained by the individual who created them for a considerable length of time (Coll & Treagust, 2003b).

She (2004) suggested that the structure of knowledge is hierarchical where concepts of higher hierarchical level subsume more essential underlying concepts. For example, She's (2002) previous research indicated that reconstructing students' conception of buoyancy requires constructions of six supplementing mental sets; therefore, misconceptions about buoyancy are difficult to change.

Within this base of knowledge, it is possible that both alternative and scientific meaning of the same concept can coexist where each associates with a different context (Chi, 1992; Mortimer, 1995; Vosniadou, 1994). Mortimer (1995) further described that learning science is not only to develop and change zones of a conceptual profile, from lower levels to more complex levels, but also to acquire consciousness of the relationships between different zones and consider which zone has higher explanatory power in a specific context or a problematic situation. According to Mortimer, each zone includes both common sense and scientific ideas, and it is epistemologically and ontologically different from other zones. Sometimes, a learner's epistemological and ontological views at the lower zone may hinder the construction of knowledge at the more complex zone.

Mortimer's (1995) theory is particularly useful to explain the use of multiple models in chemistry. The idea of conceptual profile helps to explain how students shift from one model (e.g., Bohr model of atom) to another (e.g., electron-cloud model of atom). To do so requires students to change their conceptions ontologically (because there are different ways of looking at an atom) and epistemologically (depending on the question, one model may have more explanatory power than the other). Based on Mortimer's descriptions about zones of conceptual profile, each model becomes a framework of knowledge, supported by a set of pre-assumptions and presuppositions, rather than a single, stand alone concept.

In this study, I use conceptual framework to describe an individual's base of knowledge about a specific concept, for example, molecular polarity. Conceptual framework is featured as a schema-like structure that consists of interrelated conceptual components including models and mental models. Secondly, many zones of conceptual profile about the same concept coexist (for example, the idea about a chemical single bond as a pair of shared electron versus a pair of overlapped σ orbitals from two atoms), and an individual chooses different zones to explain a phenomenon, depending on the context of a problem. Finally, a hierarchical structure features the conceptual framework that learning a concept at a higher hierarchical level requires understanding of prerequisite concepts.

Thinking with Mental Models

Mental models are intrinsic representations of objects, ideas, or processes which individuals generate during cognitive functioning (Buckley & Boulter, 2000; Harrison & Treagust, 2000). Learners use these models to reason, describe, explain, predict phenomena, and/or generate expressed models in various formats (e.g., verbal description, diagrams, simulations, or concrete models) to communicate their ideas to others or to solve problems (Borges & Gilbert, 1999; Buckley & Boulter, 2000; Greca & Moreira, 2000; Harrison & Treagust, 2000). When their mental model fails to assimilate new experiences, learners start to be dissatisfied with the existing model and may modify the model drastically or construct a different model (Glynn & Duit, 1995).

Mental models encompass propositional reasoning (Briggs, 2004) and can be either physical, which mentally represent physical entities, or conceptual, which are mental representations of concepts or abstract models (Coll & Treagust, 2003b). When the mental models are precise and coherent with scientifically accepted knowledge, for example, the models created by teachers for instructional purposes, they are called conceptual models. Some mental models which survive through rigorous experimental testing, are published in scientific literature, and become widely accepted by the scientific community are called scientific models (Coll & Treagust, 2003a; Franco & Colinvaux, 2000).

When conceptual models are introduced in chemistry classrooms, students are attempting to make sense and constructing meaning by constructing mental models based on their personal knowledge. The generated mental models then evolve and become more elaborate and often are modified by adding, deleting, and modifying concepts, features, and relationships. Glynn and Duit (1995) recommended that mental models should be considered as an important part of learners' conceptual framework.

Briggs and Bodner (2005) argued that visualization and construction of mental models serve as an important role that supplies students with a tool of thinking for model-based reasoning. They found that second-year organic chemistry students employed a set of visualization operations to make sense of an input from their eyes and to manipulate a constructed mental model to solve a problem. Five components of the visualization operations were identified including referent, relation, rules/syntax, operation, and result (Briggs, 2004). However, students do not always construct mental models when they encounter representations in the classroom. Stieff et al. (2005) indicated that secondary and post-secondary students were able to have discussions about stereochemistry by directly inspecting molecular representations without generating a mental image. Instead, the students developed some rules or strategies, such as simply looking for planes of symmetry within a molecular representation to make their decisions in a specific context. When the rule failed to provide an immediate solution, they then applied visual-spatial thinking to solve the problem. Stieff et al. claimed that this ability to alternate between the use of visualization strategies and non-imagistic heuristics increases as students' experience grows.

Sometimes students do not construct mental models due to their lack of practice with the visual-spatial ability and/or a lack of awareness about the importance of constructing mental models (Briggs, 2004). These students may draw several representations to make personal sense of a problem, yet limited by the information that static representations can provide, these representations fail to activate appropriate heuristics that lead to a correct solution to the problem (Bodner & Domin, 2000).

The two components of conceptual framework suggest that fundamental knowledge and construction of mental models play a crucial role in learning chemistry at the submicroscopic-symbolic domain. Thinking with models requires an individual to construct and use mental models based on his or her personal knowledge and sometimes to think in 3D. I believe that examining students' mental models of molecular geometry and polarity provides a window to investigate the processes of model-based thinking and the relationships among the fundamental knowledge, visual-spatial thinking, and thinking with mental models.

Definition of Terms

For this study, the following terms are defined:

Alternative framework: Alternative framework (Taber, 2001a) is a conceptual framework consisting of many sub-concepts that students apply to the framework in an inappropriate context, for example, octet framework.

Anthropomorphic explanations: "Anthropomorphic explanations involve the attribution of human traits to nonhuman beings" (Zohar & Ginossar, 1998). For example, students stated that "You have your noble gases that have that full octet: they're happy" (Nicoll, 2001, p. 715) or ions "carry" a charge (Treagust & Chittleborough, 2001).

Anthropomorphic explanations are considered as pseudoexplanations in chemical instruction.

Conceptual framework: Conceptual framework describes an individual's general background knowledge about a specific concept, for example, molecular polarity. This framework includes three features where, first, a schema-like structure consists of interrelated conceptual components including models and mental models. Secondly, it has a hierarchical structure that learning a concept at the higher level of hierarchy requires constructions of prerequisite concepts. The third feature aligns with Mortimer's (1995) description about knowledge structure that many zones of a conceptual profile can coexist about the same concept. For example, an individual can hold both ideas that a chemical bond is a pair of shared electrons and is a pair of overlapped σ orbitals from two atoms, but chooses one of the ideas for explanation depending on the context of a problem.

Chemical Bonding (CB) Instrument: Diagnostic instrument to assess students' understanding about chemical bonding. This instrument consists of seven two-tier multiple-choice items. It is an integrated two-tier multiple choice diagnostic instrument based on Peterson et al.'s (1989) two-tier test on *Bonding and Structure* and *Chemical Bonding Diagnostic Test (CBDT)* (Jang, 2003). According to Peterson et al. (1989), only about 50% of the Grade 12 chemistry students answered both parts of the two-tier items correctly for 9 of 15 items (60% of the questions were answered correctly).

Electronegativity (EN) Instrument: Diagnostic instrument to assess students' understanding about electronegativity. Taber (2002a) developed two versions of *Chemical Misconceptions – Ionization Energy Probe* to diagnose students' misconceptions about ionization energy and electronegativity. The original instrument contains 30 True/False questions, and the version used in this study is a short-version of only 20 items.

Geometry and Polarity (GP) Instrument: Diagnostic instrument to assess students' understanding about molecular geometry and polarity. This instrument combines four multiple-choice questions from Furió et al.'s (2000) *Questionnaire 2* and 11 items from Peterson et al.'s (1989) two-tier diagnostic instrument, *Bonding and Structure*.

High-scoring students: Students who have percentages of questions answered correctly ≥ 70% for two out of three diagnostic instruments. High-scoring students are individuals who possess more prerequisite knowledge about molecular polarity and had more successful performance on all three diagnostic instruments.

Low-scoring students: Students who have percentages of questions answered correctly ≤ 50% for two out of three diagnostic instruments. Low-scoring students represent students who encounter difficulties that lead to their failure in responding to the diagnostic items correctly.

Misconception: Taber's (2001a) definition of misconception describes a simple conception that is different from the domain accepted conception or from the desired outcome of teaching.

Mental models: Mental models are intrinsic representations of objects, ideas, or processes which individuals generate during cognitive functioning to reason, describe, explain, or predict phenomena (Buckley & Boulter, 2000; Harrison & Treagust, 2000). Mental models can be either physical, which mentally represents physical entities, or conceptual, which are mental representations of concepts or abstract models encompassing propositional reasoning (Briggs, 2004; Coll & Treagust, 2003b). Most of the mental models discussed in this study are conceptual mental models (e.g., a chlorine atom or a molecule of hydrogen sulfide) involving both mental representations and propositional reasoning.

Mental representations: Mental representation describes image-like information (e.g., ball-and-stick or space-filling models, stereochemical formula, Lewis dot structure, or chemical formula) in a person's mind. An individual can apply visual-spatial thinking to manipulate his or her mental representation by applying propositional reasoning in order to conceptualize a concept or phenomenon. Some students may form a mental representation but aren't able to apply visual-spatial thinking or propositional reasoning; therefore, it is important to distinguish the description of mental representation from mental model when studying students' understanding about molecular polarity.

Teleological explanations: Teleological explanations describe students' logical reasoning thinking "entities are considered as having purposes or functions that may occur beyond mechanical interactions" (Talanquer, in press). For example, students may state "every element wants a full octet, so they want eight electrons to be stable" (AM, interview). Anthropomorphic and teleological explanations are often linked to each other, and both imply goal-oriented behavior for nonhuman objects (see Zohar & Ginossar, 1998 for more detail descriptions). Teleological explanations are considered as pseudoexplanations in chemical instruction.

Two-tier multiple choice diagnostic instrument (or two-tier test): The items for the two-tier test include two parts: the first part is a multiple choice content question usually having two or three options, and the second part is the reasoning question containing a set of three or four possible reasons for the answer to the first part. The incorrect answers (distracters) are derived from students' alternative conceptions from the literature, interviews, and free response tests (Jang, 2003). For the two-tier test items, answers were considered correct when the student answered correctly both content and reasoning questions.

Visual-spatial thinking (or visualization ability): Visual-spatial thinking involves one using his/her eyes to identify, locate, and think about objects or representations, and form, inspect, transform, and maintain an image in the "mind's eye" when the original visual stimulus is absent (Mathewson, 1999). Visual-spatial thinking is closely associated with construction, recall, and retention of mental models and allows an individual to manipulate (e.g., rotate, reflect, or inverse) his/her mental model(s) to solve a problem.

Significance of the Study

The significance of the study is twofold. First, research has shown that molecular polarity is a difficult concept for students to understand (Furió & Calatayud, 1996; Furió et al., 2000; Peterson et al., 1989); and the literature focused on student understanding of molecular polarity is limited (Furió & Calatayud, 1996). These studies were conducted outside of the United States that examined students' learning difficulties associated with molecular polarity (Furió & Calatayud, 1996; Furió et al., 2000; Jang, 2003; Peterson et al., 1989). However, American students' understanding of molecular polarity and misconceptions regarding prerequisite conceptions remain unclear. The results of quantitative research in this study were valuable in identifying misconceptions for college chemistry instruction in the United States.

Previous research on molecular polarity used a quantitative phase describing students' understanding of this topic (Furió & Calatayud, 1996; Furió et al., 2000; Jang, 2003; Peterson et al., 1989). Briggs (2004) called for a new perspective to focus on the nature and process of the thinking mind. Stieff et al. (2005) also urged a coherent theoretical perspective that accounts for the role of visualization and comprehension, and new research methods that explain this relationship empirically. Consequently, a multiple-case study based on eight one-on-one interviews was used to compare students' application of their conceptual framework, external representations, and mental models to conceptualize molecular polarity problems.

To echo Briggs' (2004) and Stieff et al.'s (2005) call for new research methods and perspective, this dissertation work employed a mixed-method approach integrating quantitative and qualitative methods to investigate students' utilization of existing conceptual framework and visual-spatial thinking while solving molecular polarity problems. The findings of this study went beyond the identification of alternative conceptions in a specific domain to provide potential explanations of the connection between construction and utilization of mental models and conceptual understanding. Also, comparisons of the thinking processes between high-scoring and low-scoring students provided a rich description about the roles of external representations and mental models during problem-solving processes. Understanding the role and use of mental models in the learning process will enable chemistry teachers and instructional designers to develop strategies that foster students' comprehension about molecular polarity (Briggs, 2004).

Assumptions

To address the purpose of study and the overarching research question, the structure of the study employed a two-phase design. Phase one of the study took a quantitative approach administrating three diagnostic instruments in a general chemistry class to identify misconceptions and characteristics of the conceptual framework associated with molecular polarity. Scores of the three instruments were used as criteria to sample participants for in-depth interviews at the second phase. The results of the quantitative analysis served as a source of data triangulation for within-case analyses of interviews. This study took a mixed-method approach based on following assumptions:

Quantitative Phase

The assumptions made in first phase of the study are:

1. The sample group which is used in this study during the 2006-2007 academic year is a representative sample of the population for coeducational academic general chemistry students in the United States.
2. The misconceptions about electronegativity which Taber (2000) identified was based on the cross-institute groups in England are appropriate for the United States population.
3. The misconceptions about chemical bonding which Peterson et al. (1989) and Jang (2003) identified based on the student samples in Australia and South Korea, respectively, are appropriate for the United States population.
4. The misconceptions about molecular geometry, polarity, and intermolecular force which Peterson et al. (1989) and Furió et al. (2000) identified are based on student samples in Australia and Spain, respectively, are appropriate for the United States

population.

5. Scores of instruments EN, CB, and GP accurately reflect students' understanding on concepts of electronegativity, chemical bonding, and molecular geometry and polarity.
6. The higher the scores on the instruments CB and EN, the better the student's conceptual understanding on concepts of electronegativity and chemical bonding; the lower the scores on the instruments CB and EN, the worse the student's conceptual understanding on the concepts of electronegativity and chemical bonding.
7. Due to the nature of the concepts of molecular geometry and molecular polarity, I assumed that items in instrument GP demanded more students' ability of spatial visualization to answer them correctly. Thus the higher the score on the instrument GP, the better the student's conceptual understanding on concepts of molecular geometry and polarity and better ability to construct and use mental models; the lower the score on the instrument GP, the poorer the student's conceptual understanding on concepts of molecular geometry and polarity and the poorer the ability to construct and use mental models.

Qualitative Phase

The second phase of the study takes a personal constructivist perspective to focus on meaning-making activities in an individual's mind. As a constructivist, I believe that individuals create their sense of reality out of the information that their senses provide (Briggs, 2004). Individuals possess different levels of visualization ability. Because the fact that visualization ability is relative among individuals, even though the same 2D diagrams of molecular models or stereochemical formula are used in a chemistry classroom, students who possess lower visualization ability may perceive and construct ideas of 3D molecular structure differently from those who possess higher visualization ability.

It is assumed that people can have similar propositional knowledge yet construct different mental models. In addition, some students may have difficulties perceiving and constructing mental models from 2D representations, and/or manipulating the mental models to assist processes of thinking. This absence of mental models as tools of thinking may hinder their conceptualization of the concept to be taught.

Another assumption is that people can construct knowledge about something even when their knowledge is fragmentary or imprecise (Briggs, 2004). Research on student misconceptions has suggested that often students possess misconceptions due to their fragmented fundamental knowledge, absence of essential prerequisite conceptions, or application of inappropriate prior knowledge to conceptualize the concept to be taught (Krajcik, 1991; Mortimer, 1995; Taber, 2002a). Molecular polarity subsumes several underlying concepts including (1) periodic variation (including atomic model and valence electrons), (2) chemical bonding (including construction of a Lewis structure), (3) electronegativity and dipole moment, and (4) molecular geometry.

Based on the previous two assumptions, there are two learning impediments: (1) failure to construct and use mental models as tools of thinking and (2) missing and/or fragmented conceptual framework that have major influences on students' conceptualization of molecular polarity. It is assumed that learning the concept of molecular polarity successfully requires the understanding of its prerequisite concepts as well as being able to construct mental models to facilitate visualization and sense-making processes. These two factors determine the difference between performances of high-scoring students and of low-scoring students.

Limitations of the Study

Based on the design of study, limitations of the study are described as following:

Limitations of the Quantitative Method

1. Not all prerequisite concepts for learning molecular polarity have diagnostic test items to investigate students' misconceptions. Four concepts were considered as prerequisite knowledge of molecular polarity including (1) periodic variation (including atomic model and valence electrons), (2) chemical bonding (including construction of Lewis structure), (3) electronegativity and dipole moment, and (4) molecular geometry. Due to the diagnostic instruments available in the literature, only chemical bonding and molecular geometry were assessed by instruments CB and GP. Concepts of periodic variation, electronegativity, and dipole moment were only partially addressed by instruments EN and GP.
2. The measurement of students' understanding was limited to their scores on the three diagnostic instruments and not extended to all topics related to molecular polarity.
3. This study was limited to the participating students in the class of general chemistry and not extended to other countries and students in other grade levels.
4. Learning styles and reasoning ability of students vary greatly within the classroom. No attempt was made to control students' visual preference and reasoning skills.

5. The three instruments were administrated through an online educational system-BlackBoard that allowed students to log in and respond during the period of a week. No attempt was made to control time and condition of taking the diagnostic instruments. The time and condition that students completed the instruments may influence the results of the study.

Limitations of the Qualitative Method

Researchers need to be aware that the employed form and substance of the questioning may trigger only a particular view or form of explanation. Thus an individual's responses need to be analyzed within the context and questions he/she was asked (Borges & Gilbert, 1999; Franco & Colinvaux, 2000). On the other hand, researchers portray an individual's mental model by interpreting the expressed responses. The interpretation is mediated by the researchers' ontological and epistemological beliefs (Coll & Treagust, 2003a), thus it may be different from the idea that the individual holds (Coll & Treagust, 2003a, 2003b; Glynn & Duit, 1995; Harrison & Treagust, 1996).

The gap between what an individual expresses and what is going on in his/her mind is another issue. Therefore, speech, drawing, or writing may not reflect the entire thinking process (Eilam, 2004; Franco & Colinvaux, 2000). One reason is that the mental model is implicit to the individual who holds it; hence his or her expressed model may not represent the entire structure of knowledge about a specific concept. Coll and Treagust (2003b) also indicated that students are likely to "retreat to safer, more established positions" (p.703) when in new environments, such as interviews or exams. Thus participants' responses are likely to fall back to simple models with which they feel more comfortable or are more familiar (2003b), or attempt to comply with sociocultural norms and expectations (Coll & Treagust, 2003a).

Organization of the Dissertation

This dissertation is divided into five chapters. Chapter One provides a brief overview of research including the rationale, purpose, significance, assumptions, and limitation of the study. In addition, I present the conceptual framework that guides this study including fundamental knowledge and mental models. Chapter Two elaborates on these two conceptual frameworks by delineating how they are discussed within the research literature.

Chapter Three outlines the research approach to this mixed-method design. This includes a description of research questions and details of the context of the study including the course structure and concepts to be studied. For the quantitative phase, I describe variables, instrumentations, participants, and methods for data collection and data analysis. For the qualitative phase, I include a description of research tradition and methods for data collection and data analyses.

Chapter Four starts with findings from the quantitative phase, followed by qualitative findings on students' mental-modeling ability, level of content knowledge, and features of mental models as outcomes of interaction between mental-modeling ability and content knowledge.

Chapter Five includes summary of the study, conclusions and assertions on cross-case analyses for students' mental-modeling ability and level of content knowledge, as well as interactions between mental-modeling ability and content knowledge in relation to the research literature. This chapter concludes with implications and recommendations for future research.

CHAPTER TWO

LITERATURE REVIEW

This chapter is organized into two parts. The first part of this chapter examines the chemical education literature on methods used to investigate learners' mental models. The second part of the chapter explores literature on student understanding of concepts about molecules at the submicroscopic-symbolic domain. Learning concepts of molecular geometry and polarity in undergraduate chemistry curriculum draws heavily upon knowledge at the submicroscopic and symbolic levels. Learning difficulties associated with concepts of molecular geometry and polarity as they relate to students' difficulties on prerequisite concepts at the submicroscopic-symbolic domain.

Methods Used to Investigate Learners' Mental Models

Mental models are generally described as incomplete, imprecise, influenced by individuals' beliefs, and evolving through interaction with a concept or phenomenon to be represented (Greca & Moreira, 2000; Harrison & Treagust, 1996). Franco and Colinvaux (2000) summarized four characteristics of mental models including:

- Mental models are generative: Mental models can lead to new information through utilizing them to predict and to generate explanations.
- Mental models involve tacit knowledge: Individuals reason with their mental models to solve a problem or make sense of new information, but they may not be aware of the mental models they hold and how they use them.
- Mental models are synthetic: A mental model is dynamic and continuing to be modified as new information is incorporated into it.
- Mental models are constrained by world-views: The development and application of

mental models is influenced by individual's prior knowledge, experience, and beliefs.

Individuals' mental models are commonly investigated through interpretations of their expressed models or verbal explanations (Buckley & Boulter, 2000; Franco & Colinvaux, 2000). Data sources of the expressed models include: material productions, such as student notebooks (Scott, 1992), scientists' diaries (Franco & Colinvaux, 2000), learner-constructed diagrams (Coll & Treagust, 2001, 2002, 2003a, 2003b; Harrison & Treagust, 1996, 2000; Lichtfeldt, 1996; Scott, 1992; Taber, 2003a; Williamson & Abraham, 1995), scientists' published papers (Franco & Colinvaux, 2000), preference of pictorial or concrete models (Coll & Treagust, 2001, 2002, 2003a, 2003b; Harrison & Treagust, 1996, 2000; Lichtfeldt, 1996), short-answers or essay to a presented problem (Eilam, 2004; Williamson & Abraham, 1995), and oral descriptions obtained in interviews (Chiu, Chou, & Liu, 2002; Coll & Treagust, 2001, 2002, 2003a, 2003b; Harrison & Treagust, 1996, 2000; Scott, 1992; Taber, 2003a). Because of the nature of the complexity of mental models, most of the studies utilized multiple data sources to portray learners' conceptual frameworks from various aspects. Table 1 summarizes the instruments used to study mental models in the literature of chemical education. Common instruments used in the studies of mental models include multiple-choice questions, open-ended questions (with drawings and descriptions), interviews with probing questions (often supplemented with drawings and descriptions from the interviewee), interviews with pictorial or concrete models to elicit their preferred models, interviews with problems presented, and classroom observations.

Two-Tier Diagnostic Instruments

Having a different purpose than assessing students' summative learning outcomes,

Table 1

Researches on Mental Models in Chemical Education

Research Instruments / Studies on mental models	Paper-pencil responses		Interviews			Class observations	Others
	Multiple-choice questions	Open-ended questions	With probing questions	With given pictorial or concrete models	With problems or phenomena		
Mental model of atoms and molecules, Grade 8, 9, 10 (Harrison & Treagust, 1996)			+	+		+	
Effect of computer animation on particulate mental models, post instruction, college chemistry (Williamson & Abraham, 1995)	+	+					
Mental model of the nature of matter, post instruction, Grade 7 (Eilam, 2004)					+		
Chemical equilibrium, post instruction, Grader 10 (Chiu et al., 2002)				+	+		
Mental models of chemical bonding, cross-age study, Grade 12, undergrad, and postgrad (Coll & Treagust, 2001, 2002, 2003a, 2003b)			+	+	+		Analysis of curriculum materials
Ideas about atoms, longitudinal study, Grade 7 through 11 (Lichtfeldt, 1996)	+	+				+	Word association
Structure of matter, longitudinal study, 14 year-old (Scott, 1992)		+	+				Diary keeping
Mental model of metals, longitudinal study, college chemistry (Taber, 2003a)			+	+		+	
Mental model of atoms, molecules, and chemical bonds, longitudinal study, Grade 11 (Harrison & Treagust, 2000)			+	+		+	

+: The instrument is used in the corresponding research.

diagnostic instruments are developed to elicit learners' misconceptions related to a specific concept. The development of diagnostic instruments has focused research on students' concepts and misconceptions, in particular content area, provide practical assessment for two reasons. First, a teacher can use diagnostic instruments to elicit students' existing knowledge as a starting place for instruction. Second, researchers can administer the instruments to a large student sample when interviews are less practical (Treagust, 1995).

The heuristic power of a diagnostic instrument is dependent on its ability to externalize a student's responses and reasons when solving problems about a specific concept. Traditional, multiple-choice instruments have difficulties uncovering misconceptions because the reasons for students' wrong answers are not identified (Griffard & Wandersee, 2001). The format of two-tier diagnostic items was used to identify students' alternative conceptions in limited, clearly defined content areas (Chiu, 2007; Jang, 2003; Peterson et al., 1989; Tan & Treagust, 1999; Treagust, 1995; Treagust & Chandrasegaran, 2007). Each two-tier diagnostic item consists of two parts: the content part and the reason part. The first tier of the item identifies a student's response to a content question, and the second tier elicits the student's reason for his or her answer. The distracters at the second tier (the reason part) are students' conceptions and/or misconceptions identified in the literature and gathered from student interviews or open-ended surveys conducted during the developmental stage of the diagnostic instrument. The development of a two-tier diagnostic instrument goes through procedures of defining content and associated concepts and gathering information about students' alternative conceptions. Once the diagnostic instrument is crafted, it is piloted, refined, and tested for reliability (see Treagust & Chandrasegaran, 2007 for details about development of two-tier diagnostic items). Treagust and Chandrasegaran summarized the diagnostic instruments developed since the 1980s. Among 21 published studies, eight of them addressed chemistry concepts on covalent bonding and structure, chemical bonding, oxidation and reduction, chemical equilibrium, multiple representations in chemical reactions, ionization energies, acids and bases, or states of matter.

Two-tier diagnostic instruments provide researchers a validated tool to elicit students' understanding and misconceptions, Griffard and Wandersee (2001) caution that there are some issues a researcher needs to be aware of when interpreting data from the diagnostic instruments. Griffard's and Wandersee's study investigated how six upper level college biology students approached a two-tier instrument about photosynthesis using a think-aloud technique. Their findings indicated that raw scores on the two-tier diagnostic items may have underestimated students' knowledge when students who looked for deeper meaning in an item chose a distracter. In other situations, the results of two-tier items may not reflect students' knowledge. For instance, students may rely on logic or identifying scientific terms to make a correct choice, rather than applying their existing knowledge to answer the question. Moreover, the researchers indicated that each participant considered the reason part as a distinct question, and then finalized their choice thinking whether it logically followed their response to the content part. According to Griffard and Wandersee, the two-tier instrument seems to measure a student's test-taking skills rather than the existing knowledge.

Griffard and Wandersee (2001) also commented that the instrument on photosynthesis, designed for secondary students, was oversimplified when given to upper college biology level. Due to the variations in grade level, content of textbooks, instruction, and use of language/symbols in the classroom among student populations, types and sources of students' misconceptions may vary; therefore, items or wordings of the diagnostic instrument may need to be modified for different student populations.

When applied in an investigation of mental models, multiple-choice, diagnostic items require researchers to puzzle and interpret learners' responses to a series of questions to reveal their views about a specific concept. When investigating students' understanding of an advanced concept, the items actually diagnose isolated, discrete misconceptions in a student's conceptual framework, rather than revealing missing propositions that form connections between conceptions (Griffard & Wandersee, 2001).

Open-Ended Responses

In general, the way that open-ended responses are formatted is similar to the questions in the interviews. One weakness of using questions in a paper-pencil format is that they rely on students' willingness to provide rich information. A paper-pencil format does not allow researchers to probe further when students' answers or the reasons for the responses are not clear. However, both multiple-choice questions and open-ended responses can be used to elicit students' initial ideas to provide cues for developing interview questions. Most of the investigations on mental models utilized interviewing as the main data source because it allows a dynamic interaction between the interviewer and the interviewee. The interviewer is able to probe further or to adjust questions based on the interviewee's responses; it also helps to examine the meaning of learners' languages, either the everyday language or the scientific terms (Scott, 1992).

Probing questions, models (pictorial or concrete), or problems are usually incorporated in interviews to examine how learners use their mental models to interpret new information and to predict and explain in various situations. In the next three sections, I will give examples of how the three methods were used with interviews to investigate mental models.

Interviews with Probing Questions and Drawing

Interviews allow researchers to elicit learners' mental model of a target system (e.g., the structure of an atom or chemical bonding) by using probing questions. Researchers are able to probe for the details of mental models, for example, asking learners to describe their idea of "sea of electrons" while describing metallic bonding (Taber, 2003a), or asking them how far the electron cloud extends out from the nucleus of an atom using a 5-cm-diameter polystyrene ball to represent the nucleus as an aspect of individuals' mental model about an atom (Harrison & Treagust, 1996). Probing for word association, for example, by asking learners to write down the words associated with "atom", is another useful extension (Kleinman, Griffin, & Kerner, 1987; Lichtfeldt, 1996). Drawings and interviewing often go hand-in-hand because they allow learners to express their mental model with few limits on how they may respond. The precision and sensitivity can be increased greatly when a drawing can be supplemented within the interview by asking why the learner drew or wrote something in a particular way (White & Gunstone, 1992). An application is to elicit learners' expressed model directly from a drawing of what they think a phenomenon looks like on a very small scale, for example, drawing an atom or a water molecule (Coll & Treagust, 2001, 2002; Harrison & Treagust, 2000; Lichtfeldt, 1996) or the particles in gases, liquids, and solids (Scott, 1992; Williamson & Abraham, 1995). However, a limitation is that some students may prefer and feel less pressure to provide their explanations verbally without drawing.

Interview Using Pictorial or Concrete Models for the Selection of Preferred Models

An alternative way to probe for learners' understanding of a specific model or concept is to ask them to choose their preferred models from a series of models they have seen or been taught in the classroom. Model selection involves an examination of textbooks and instructional materials to decide which models are used in the interview. Learners are asked to indicate the model(s) that best fit their mental model or least appeal to them, for example, choosing between space-filling and a ball-stick molecular models for H_2O (Harrison & Treagust, 1996), and choosing among models of atoms (Coll & Treagust, 2001; Harrison & Treagust, 1996), or models of bonding (Coll & Treagust, 2001, 2002, 2003a, 2003b). Learners are also probed for the reasons behind their choice. Figure 2 gives an example of the models that were used in a study on mental models about metallic bonding (Coll & Treagust, 2003b). Sometimes concrete models were used, for example, giving learners a polystyrene ball and a pompon (with a hard center) and asking them if either of these models share any similarities with their idea of an atom (Harrison & Treagust, 1996).

Interview with a Problem Presented

Methods in the previous two sections focus on capturing the content of learners' mental models (Harrison & Treagust, 1996; Taber, 2003a). To examine how learners use their mental models to predict and to explain when a problem or a phenomenon is presented, two methods are often seen in the literature: Interview-about-events (IAE) and Prediction-observation-explanation (POE).

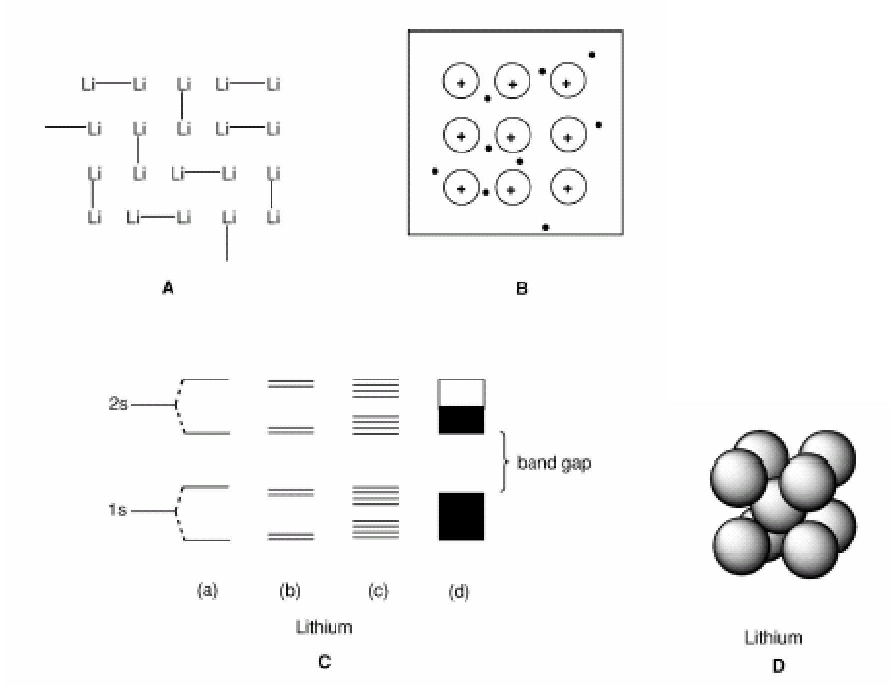


Figure 2. Models for metallic bonding used in Coll's and Treagust's study (2003b).

Interview-about-events (IAE). The IAE technique probes for learners' understanding of a specific concept by initiating interview questions using one or a series of diagrams. Learners are shown IAE focus cards depicting problems or phenomena that require them to evaluate the conditions of the problem, to reason through the context, and to come up with the explanations which make sense with their mental model. For example, to reveal how college students developed an idea about metallic bonding based on their prior learning on chemical bonding, Taber (2003a) explored students' mental models by asking them to interpret a representation of iron particles in a lattice arrangement and to answer whether bonding was shown in the substance/species. By the end of a two-year course, some students did not let go of their initial idea and still believed that there is some form of interaction in metals, but not proper bonding. Other students held various mental models about metals having covalent bonding, ionic bonding, or both of them, or some kind of similar bonding. Students also held a wide range of ideas about the conceptualization of the “sea of electron” metaphor. In another study on mental models about metallic bonding, participants needed to explain the conductivity of a copper wire by comparing it with a glass rod and to explain its malleability (Coll & Treagust, 2003b). The results indicated that learners were able to provide fluent descriptions of some familiar conceptual models, for example, a sea of electrons model; however, their abilities to understand and to explain the represented events on IAE focus cards were limited (Coll & Treagust, 2001, 2003b).

Another application of IAE is to present problems by asking learners to draw explanations for a series of changing situations. Scott (1992) explored a secondary student’s microscopic view about solids, liquids, and gases through drawings and explanations of her reasons in different contexts. For example, the student had to explain why a syringe full of water could not be compressed, but a syringe full of air could be compressed. She was also shown a flask connected to a vacuum pump and was asked: “If you were able to see the air in the flask, draw how it would look before and after the vacuum pump was used to remove some of the air?” (p.208). Some probing questions could follow to probe for the individual’s drawing (e.g., What is in between the particles? Do the particles sit still or keep moving?). Using similar problems and interview questions throughout the semester, the results indicated that the learner experienced a number of stages before she reached a more scientific view. In addition, some alternative conceptions were generated during the process of reasoning.

Prediction-observation-explanation (POE). The POE technique probes for learners’ understanding by requiring them to first predict an outcome of some events and to provide reasons. After the event is demonstrated, they then describe what they saw happen, and finally reconcile any conflict between prediction and observation and justify their explanation. White and Gunstone (1992) indicated that a prediction is more likely to require the respondents to use their knowledge to reason an answer rather than to reproduce textbook knowledge without thinking. This technique allows researchers to investigate not only the respondents' explanations based on his/her mental model, but also what conditions of the event that he/she believes need to be considered. Chiu et al. (2002) utilized a series of POE events to investigate secondary students' mental models of chemical equilibrium. For example, they asked students to predict and to provide reasons for "What would be observed if we put a tube of $Co(H_2O)_6^{2+}{}_{(aq)}$ solution into hot water?" While the learners described their observations and explanations during the demonstration, some guiding questions may follow, such as "Is it a physical change or chemical change? Why?", "What kind of equilibrium occurs?", or having them discuss what factor influences the chemical reaction. A schematic diagram was then developed to portray students' knowledge structures of chemical equilibrium before and after the instruction. In physics, POE was used to assess learners' mental models of electricity by asking them to light a light bulb with two wires and a battery and to provide reasons for why it works (Borges & Gilbert, 1999).

To elicit students' understanding about molecular polarity and prerequisite concepts for a large student number, I used three diagnostic instruments, adopted and modified from previous literature (details about content and implementation of the diagnostic instruments will be discussed in Chapter Three) in this study. To reveal participants' perceptions about chemistry principles and chemical representations as well as their application of existing knowledge during the interview, I developed a set of thought-revealing tasks based on literature of diagnosing student misconceptions about atoms, molecules, and chemical bonding (detail descriptions about the design of interview protocol was discussed in Chapter Three). I also provided play-sough and straws and encouraged students to construct concrete models during the interview in order to reveal students' mental models containing spatial information of 3D molecular structures.

Learning Impediments at the Submicroscopic-Symbolic Domain

In the second part of this chapter, the review of literature was organized based on factors that may explain the learning impediments at the submicroscopic-symbolic domain. Three main learning impediments were identified in the literature: (1) a lack of integrated conceptual framework, (2) commonsense reasoning, and (3) insufficient understanding about chemical representations and models.

A Lack of an Integrated Conceptual Framework

Tremendous evidence has been found to support a constructivist perspective on learning (Bransford, Brown, & Cocking, 1999; Donovan & Bransford, 2005; Driver, Squires, Rushworth, & Wood-Robinson, 1994). It is now widely accepted in the science education community that a learner's existing conceptual framework can provide the bedrock on which new ideas are anchored. While appropriate conceptions provide a stepping stone to a new understanding, incorrect, low quality, missing, or fragmented knowledge can act as barriers (Taber, 2003b).

Taber (2002a) and Ringnes (1994) each attempted to understand how the lack of an integrated conceptual understanding can hinder learning in chemistry. Ringnes developed a typology of learning impediments focusing on characteristics of a knowledge base (e.g., missing knowledge elements or links between them) and misunderstanding.

Taber analyzed learning impediments from an approach of diagnosing potential misconceptions to provide information for improving instruction. The comparison between Taber's and Ringnes's typology and the examples of these learning impediments are summarized in Table 2.

According to Taber (2002a), four types of impediments were identified under two categorizations: (1) null learning impediments, which refer to the cause of not understanding, including deficiency learning impediment and fragmentation learning impediment and (2) substantive learning impediments, which indicate the cause of misunderstanding, including ontological learning impediments and pedagogical learning impediments. A null learning impediment describes the situation where learners fail to understand a new concept due to their lack of the prerequisite knowledge (deficiency learning impediment). Or they may hold the prerequisite knowledge, but do not perceive its relevance, so the new concept becomes unrelated fragments and fails to connect to the existing conceptual framework (fragmentation learning impediment).

Many misconceptions identified in the literature are categorized under null learning impediments. In a study on comparing 10 chemistry lecturers' and 88 preservice chemistry preservice teachers' understanding about chemical reaction in Singapore, Lee (1999) found that 50 % of the preservice chemistry teachers thought that the magnesium lattice and oxygen gas molecules formed either free atoms or ions before they reacted with each other. Some reacting criteria such as the short life span of intermediates as free atoms or ions were missing in their knowledge base. Therefore, it was difficult for these preservice teachers to conceptualize the interaction between magnesium lattice and

Table 2

A Comparison of Taber's (2002) and Ringnes's (1994) Typology of Learning Impediments

Taber's (2002) typology	Ringnes's (1994) typology	Students' difficulties in the literature at the submicroscopic-symbolic domain
Null learning impediment - Deficiency impediment	1a. Knowledge element missing	• When Grade 8-10 students were asked about concepts of atoms and molecules, only 27% and 50% of them were aware of concepts of electron shells and electron clouds, respectively. Sixty percent and 35% of the participants, respectively, were not aware of these two attributes of atomic model (Harrison & Treagust, 1996). • Some students ignore that, in using VSEPR theory, a multiple bond should be treated as through it was a "single" electron pair (Furió & Calatayud, 1996, p. 38).
	1b. Low level, or one level of knowledge	• Students lack the differentiation of (or confused by) similar concepts such as the arrangement of electron pairs vs. molecular shape when constructing a molecular structure. (Furió & Calatayud, 1996). • Freshman-level general chemistry through senior-level physical chemistry students do not understand the trend of atomic size and are confused about the trends of ionic size and electronegativity in the Periodic Table (Nicoll, 2003, p. 211).
- Fragment impediment	2. Binding between knowledge elements or between representation incorrect	• First year chemistry students posses misconceptions that the contents of the bubbles in boiling water are hydrogen and oxygen gas or believe that breaking of H-H and O-O bonds releases energy. Students do not conceptualize the levels of strength for the attractive force between H and O atoms in a water molecule (covalent bonds) and between molecules (hydrogen bonds and van der Waal's force), nor understand the amount of energy associated with the bond formation and bond-breaking. (Mulford & Robinson, 2002).
Substantive impediment - Ontological impediment	3. Misconception: Ideas conflicting with scientific theories	[Note: Because students' misconceptions may be attributed from other sources of learning difficulties, Ringnes's definition was too general. When discussing misconceptions at macroscopic-submicroscopic domains, it aligned with Taber's ontological impediment.]
- Pedagogical impediment	4a. Wrong algorithm or over-generalization applied 4b. Representation of knowledge restricted	[Note: This impediment is referred to procedural difficulty as functional fixedness or reduction.] • Teachers only present the beginning reactants and the end product of reaction (e.g. $Mg_{(s)} + O2_{(g)} \rightarrow MgO_{(s)}$) but leave the mechanism for students to reason (Lee, 1999, p. 1011). Thus students associated the heating for the chemical reaction as responsible for forming ions by relating their prior knowledge about magnesium oxide as an ionic compound. • Other difficulties due to low visual thinking ability (see Wu & Shah, 2004 for details).

oxygen gas molecules as reactions between molecules involving intermediates, rather than between free atoms or ions

A substantive learning impediment describes the situation when learners misconnect the new concept to their existing understanding or interpret the new concept in an inappropriate context. According to Taber (2002a), ontological learning impediments are due to the inconsistency between the introduced concept and the learners' everyday experiences. Pedagogical learning impediments are the misconceptions developed from the way the new concept is taught, due to the learners' misinterpretation of instructional representations, the complexity of the presented materials overloading students' working memory, or the large logical steps in the instruction for the learners to construct the teacher's meaning.

An example of substantive learning impediments includes students overgeneralizing the octet rule when determining the formation of possible substances. About 62% of Grade 12 chemistry students applied the octet rule to determine that "the substance NaH cannot exist because both Na and H are in group I with one electron in the outer shell" (Ringnes, 1994, p. 106). The octet rule is one of the important models are introduced in the early stages of chemical instruction. However, it is evident that many misconceptions can occur if the criteria for model application and its limitations are not addressed. Taber provided suggestions for addressing students' learning impediments in the classroom.

Based on students' cognitive structure, Ringnes (1994) categorized students' learning difficulties into:

1. missing or fragmented knowledge, including knowledge element(s) missing and binding(s) between two or more knowledge element missing;

2. incorrect knowledge, which involves ideas in conflict with scientific theories or facts,
3. wrong algorithm or over-generalization applied, and incorrect bindings between knowledge elements or between representations; and
4. low quality knowledge, which indicates the learning difficulty may be due to a lack of differentiation between similar concepts, a lack of clarification of the criteria for applying the concept or principle, or the understanding that only takes place in one level of representation.

In general, Ringnes's (1994) typology to some degree is aligned with Taber's (2002a) categorizations, except that Taber did not account for low quality knowledge. Among these impediments, ontological impediment is crucial in particular when the submicroscopic concepts are introduced to the learners.

Common Sense Reasoning

The common sense approach describes explanations about a natural phenomenon that individuals develop based on their intuition and broad generalization, or shortcuts of reasoning procedures that learners learn from experiences to make inferences with less efforts (Talanquer, 2006). Naïve learners often follow or apply the common sense approach unconsciously when a problem is encountered. One source of learning impediments is flaws in students' reasoning heuristics including functional reduction and functional fixedness. Another source of common sense reasoning results from uses of anthropomorphic terms in chemical instruction.

Functional reduction and functional fixedness. Furió's and Calatayud's (1996) and colleagues' (2000) research employed a set of multiple-choice questions to examine Grade 12 and university Spanish students' understanding about molecular geometry and polarity. Their results indicated that the students showed a tendency to reduce factors affecting molecular polarity by (a) assuming that polarity of molecules depends only on shape, while neglecting the consideration of atoms attached to the central atom ("geometric functional reduction") or (b) assuming that molecular polarity depends only on the electronegativity difference between atoms forming each bond in the molecule ("bonding functional reduction"). Furió and Calatayud attributed these students' errors to functional reduction and functional fixedness. Functional reduction describes students' reduction of the intrinsic complexity of problems during the process of reasoning. Students may reduce the number of variables when considering a task that involves two or more variables. For example, 53%, 40%, and 26% of Grade 12, first-, and third-year university students, respectively, showed geometrical functional reduction explicitly when explaining steps to determine whether a molecule is polar or non-polar (Furió et al., 2000). In Peterson and Treagust's study (1989), Grade 12 chemistry students assumed that the shape of molecules is determined by bond polarity (27%), or only due to the repulsion between the bonding electron pairs (25%), or the repulsion between the nonbonding electron pairs (27%). Thirty-four percent of the participants thought that non-polar molecules form when the atoms in the molecule have similar electronegativities. Other examples of functional reduction include students who focused on only one or a few features and ignored others while interpreting submicroscopic and symbolic representations. In Nicoll's (2003) study, while university students constructing free-form models to represent a molecular structure using play dough and straws, they did not indicate different types of bonding, and only a few considered the bond length and the relative size of atoms. When students represented single and multiple bonds in their models, the strength of the bonding was often neglected.

Functional fixedness describes the situation where students reason a chemical concept based on common sense evidence without considering their scientific knowledge. Grade 12 and first year university students drew two-dimensional Lewis structures correctly, but derived the molecular shape directly without considering the lone-pair electrons and the spatial solutions (Furió & Calatayud, 1996). Some students determined or interpreted chemical formulas without considering the oxidation number or the placement of reactants in the Periodic Table (Kousathana & Tsaparlis, 2002; Ringnes, 1994). Kousathana and Tsaparlis believed that these types of errors were due to students' hastiness, thoughtlessness, or students' working memory was overloaded by the way the question was presented.

Use of anthropomorphic terms in chemical instruction. One source of common sense reasoning results from the use of metaphorical and anthropomorphic terms in chemistry classrooms. For example, students stated that "You have your noble gases that have that full octet: they're happy" (Nicoll, 2001, p. 715). Students construct their scientific understanding through negotiating the meaning of chemical terminologies and redefining the common language through instructional guidance and peer interaction. Language is the tool for communicating the social-constructed meaning. However, it can be misused by the teacher or misinterpreted by the learners which results in misconceptions. Sources of misuses and misinterpretations of chemical terms in the classroom included the use of metaphorical words, such as donated, shared, and accepted electrons to form chemical bonds and the anthropomorphic use of language in chemical explanations such as ions "carry" a charge (see Treagust & Chittleborough, 2001 for a more detailed discussion).

Insufficient Understanding for Chemical Representations and Models

Understanding chemical representations and models is crucial for learning chemistry. In this section, four impediments to students' insufficient understanding for representations and models are summarized. These four learning impediments are: (a) lack of appreciation about role of models, (b) abstraction and unfamiliarity with symbols, (c) difficulty with shifting between/among chemical representations, and (d) a low visual-spatial thinking ability. These impediments may not occur alone during the learning processes, and the interactions between and among these impediments is not clear.

Lack of appreciation about role of models. Models of atoms, molecules, and chemical bonds are entities created by scientists as tools of thinking and of communication at the submicroscopic level to explain phenomena that are observed at the macroscopic level. Scientists use various models of the same concept, from simple and concrete to complicated and abstract, depending on the context or problems. When these models are introduced in textbooks and discussed in class, pupils generally develop a very simplistic notion of the role of models in science (Taber, 2001a).

Grosslight et al. (1991) and Harrison and Treagust (2000) studied changes of students' views about models overtime. In Grosslight et al.'s study, three levels of modeling ability were identified and revealed different epistemological views about the relationship of models to reality and the use of models in science. Many seventh graders possessed modeling ability at Level 1, in which they viewed models as simple copies of real-world objects. They believed that the purpose of a model was to mimic a real object rather than seeing the purpose underlying the model. Students may consider a model to be wrong because it did not provide enough information about reality. Students at Level 2 realize that the purpose of a model determines the way the model is constructed. Level 2 students accepted the idea that there can be different models to capture different aspects of the reality, but they did not see the use of models to portray ideas or theories. In addition, Level 2 students considered the purpose of testing a model was to examine its functions and appropriateness rather than testing the underlying idea. All experts were categorized as Level 3 who saw models as explanatory tools for developing and testing ideas. These experts believed that there should be multiple models developed and used for specific purposes. Moreover, models can be manipulated to generate new information through the cycles of construction and evaluation (Grosslight et al., 1991). This same progression about the role of models progressing from Level 1 to Level 3 was also observed in a year-long study on a Grade 11 chemistry students' mental models about atoms, molecules, and chemical bonds (Harrison & Treagust, 2000).

Abstraction and unfamiliarity with symbols. Research indicates that students have difficulties in interpreting chemical equations (Krajcik, 1991) and describing the meaning of symbols (Ardac & Akaygum, 2004). Students frequently use symbols without understanding them and balance chemical equations as if solving mathematical puzzles without understanding the phenomena conceptually (Ben-Zvi, Eylon, & Silberstein, 1987). Ben-Zvi et al.'s (1987) study indicated that about a quarter of the Grade 11 students represented the compound Cl_2O as consisting of two fragments: Cl_2 and O. When students were asked to represent the meanings of two chemical equations: (1) $2KF(l) \rightarrow 2K(s) + F_2(g)$ and (2) $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$ by drawing, 23% of Grade 10 participants were categorized as lacking understanding about chemical equations. The symbolic language does not become easier when students enter the university level. For instance, 44% of undergraduate students showed at least some confusion about the use of subscripts and coefficients when converting a particulate picture for a chemical reaction into a balanced chemical equation (Mulford & Robinson, 2002). This may be due to students' misunderstanding of symbols or to the unfamiliarity with the symbolic formalisms. Marais and Jordaan (2000) indicated that first year college chemistry students had more difficulty with meanings of symbols than with the meanings of words. Without understanding the composition of atoms, molecules, and the structure of matter, students may see formulas as merely abbreviations for names of substances rather than as a way to represent the composition of a structure (Wu & Shah, 2004). A example of misconceptions due to the lack of submicroscopic understanding in the literature is that Grade 12 chemistry students who represented hydrogen in a chemical reaction by H_2 as well as by H and H^+, neglecting the differences among molecules, atoms, and ions (Ringnes, 1994). In another example, high school students viewed $Cl_{2(g)}$ as a representation of one particle instead of a collection of a large amount of Cl_2 molecules in a gaseous state (Wu & Shah, 2004).

Difficulty on shifting between/among chemical representations. When students progress through academic levels, they are exposed to more sophisticated and abstract models. For example, in Cokelez's and Dumon's (2005) study, an atom is presented as a sphere in the Grade 8 French science curriculum. In Grades 9 and 10, students are exposed to a model of a neutral atom where the number of negative charges of electrons is equal to the number of positive charges of the nucleus. Later some Grade 10 and 11 curricula included a probabilistic representation of the electron cloud model or Bohr model. Symbolic representation, such as Lewis dot structure, is considered an abstract concept that is usually introduced at Grade 11 or 12. Gradually, students adapt new models, yet are unable to master the explanations of these more abstract models. In a cross-age study of French students' (Grade 10, 11, and 12) understanding of representations of atoms and of molecules, Cokelez and Dumon reported that 61% of the Grade 10 students used a simple sphere to represent an atom. After Lewis dot representation was introduced in Grade 11, 26% of Grade 11 students and 34% of Grade 12 students preferred using symbols with Lewis dot structure to represent an atom. The Grade 11 and 12 students who still preferred a simple sphere for an atom was reduced to 31% and 30%, respectively. Fifty-three and seventy-five percent of Grade 11 and 12 students, respectively, did not use or provided erroneous answers while using a more abstract model to represent an atom. Only 13% and 10% of Grade 11 and 12 students, respectively, indicated a model of neutral atom (the number of protons equals the number of electrons). There were similar findings when students were asked to draw a water molecule. Fifty-six and fifty-four percent of Grade 11 and 12 students drew the water molecule as a Lewis structure, yet most of the students either provided erroneous descriptions or no answer, or simply indicated that water molecule is made of two atoms of hydrogen and one atom of oxygen. Only 7% students in Grade 11 and 5% in Grade 12 mentioned covalent bonding between hydrogen and oxygen atoms.

Taber (2001b) argued that students' conceptual development is a gradual shift of the preferred choice between several alternative explanatory principles (or models) as they progress through academic levels and are exposed to more sophisticated models.

Students may simultaneously hold several explanatory conceptual schemes for a particular concept. Over time, when students undergo conceptual revolutions, their cognitive structure comes to favor the growth of a new alternative scheme that has more explanatory power (e.g., Coulombic forces) over the naïve idea (e.g., octet rule). Findings of Coll's and Treagust's (2001) study on Grade 12, undergraduate, and postgraduate Australian students' mental models of chemical bonding support Taber's argument. Coll and Treagust reported that all six participants across different academic levels preferred simple or realistic mental models for chemical bonding. When their (particularly the senior level learners) simple models were unable to explain or solve a given problem, they utilized concepts from other more sophisticated models or related to more abstract models only in the context of tests or examinations.

However, the majority of students still experienced difficulties shifting between or among chemical representations while solving a problem. For example, many Grade 8 chemistry students used one molecule to represent a collective entity in a chemical reaction system (Ardac & Akaygum, 2004). Similarly, only about 10% of the students represented $O_{2(g)}$ by many scattered molecules of oxygen (Ben-Zvi et al., 1987). Ardac and Akaygum attributed this misconception to students' difficulties in reconciling different representations of the same conception as a meaningful group or a lack of attempting to check the accuracy of representations using the available declarative knowledge.

Types of representations received and used by learners also influence their problem-solving processes. In a study of first and second year graduate students using a two-dimensional nuclear magnetic resonance spectroscopy (FT-NMR) to determine the structure of an unknown molecule, Bodner and Domin (2000) examined the number and types of representations constructed by both successful and unsuccessful problem solvers. The successful problem solvers constructed more representations per problem than their counter cohort constructed. Most representations that the successful problem solvers constructed were symbolic, compared to unsuccessful problem solvers who relied on verbal descriptions, such as "the number of spin orientations of a spin-active nucleus is equal to two times the spin-quantum number plus one" (p. 28). They also found that students who were not able to spontaneously switch from one representation (e.g., chemical formula) to the other (e. g., Lewis structure) tended to perform poorly in organic chemistry. In contrast, students who do well in organic chemistry can switch back and forth between these representation systems as needed. Bodner and Domin suggested that this difference may be due to individuals' construction of mental representations.

Shane and Bodner (2006) had similar findings that students who perceived representations of Lewis dot structures as verbal-linguistic representations tended to see these structures as collections of letters, lines, and dots rather than conceptualizing the symbols as representations of atoms and molecules. These students' descriptions about chemical phenomena tended to be static and relied on surface features of the verbal-linguistic representation. For example, when they explained a Lewis acid-base interaction, they associated the positive and negative signs of Lewis acid and base with the gain and loss of electrons without considering that as positive and negative charges of molecules. Coll and Treagust (2003a) explained the difference between successful and unsuccessful problem solvers in terms of the differences of their mental models.

Experienced chemists tend to suppress the associative image in mental models. The mental models that chemists hold are abstract ideas, generated based on the problem to solve, whereas undergraduate learners conceptualize more by word association.

From an instructional perspective, such difficulties to shift between or among representations may result from the impediments during processes of semiosis (interpretation and meaning-making) between inscriptions that depict different representations (Roth, Pozzer-Ardenghi, & Han, 2005). With different representations, for example, Lewis structures and corresponding diagrams that show relative sizes of bonding pairs and lone pair electrons (Figure 3), are presented simultaneously in the textbook or lecture, students do not always make connections between them automatically. In a study on the function and the structure of chemical inscriptions in middle school science textbooks, Roth et al. noted that different types and functions (structure) of inscriptions that constitute different signs were difficult for students to understand. Their findings on chemisemiotic analyses added to our understanding on learners' cognitive work that is required for interpreting inscriptions:

1. Reading an inscription such as Figure 3 requires an understanding of several presuppositions (e.g., understand that the dashed lines of the Lewis structures [schematic representations] represent bond axes behind the plane of the paper and the wedged lines represent bond axes in front of the plane of the paper; understand the relative sizes of binding pairs and lone pairs representing the strength of repulsive forces among electron pairs).
2. Reading an inscription requires students to organize the information within it and across other inscriptions and texts. Tremendous amount of work is involved in

learning from the inscriptions including structuring each inscription and text (caption), transposing inscriptions, linking (translating) inscription with text, and interpreting the meaning of them.

3. Surface features of inscriptions (such as color, shape, and background) may restrict the reading process. Novice students tend to focus on surface features (e.g., color) of inscriptions rather than the underlying concepts. Therefore, the instructional material becomes a potential source of students' conceptual difficulties or misconceptions in science learning.

Briggs and Bodner (2005) suggested that abilities of visual-spatial thinking and construction of mental models should be considered when studying model-based reasoning.

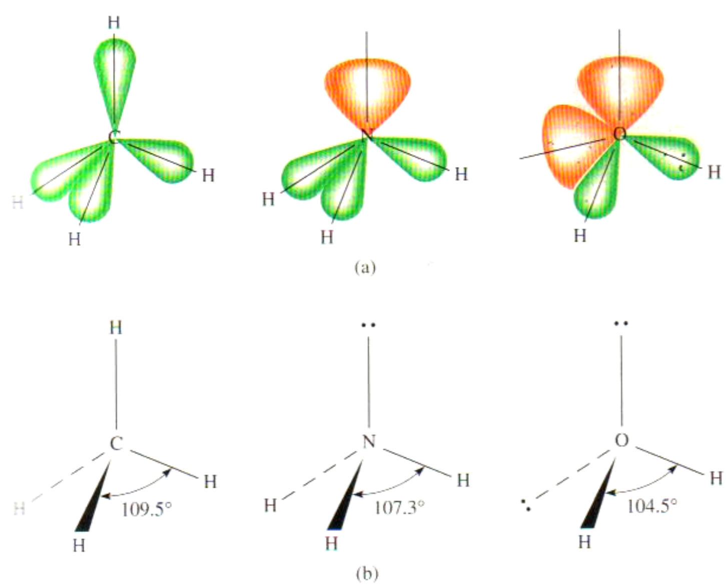


Figure 3. An example of inscriptions from a freshman chemistry textbook (adopted from Chang, 2005, p.391).

A Low Visual-Spatial Thinking Ability

Students' misconceptions at the submicroscopic-symbolic domains frequently involve visual-spatial thinking. Students' deficiency of visual-spatial thinking may hinder their formation of three-dimensional (3D) mental images by visualizing two-dimensional (2D) representations, or visualizing dynamic movement of a particulate model from a static representation (Wu & Shah, 2004).

Visual-spatial thinking, sometimes called visualization ability, involves the use of an individual's eyes to identify, locate, and think about objects or representations, and forms, inspects, transform, and maintain an image in the "mind's eye" when the original visual stimulus is absent (Mathewson, 1999). Visualization skills are further categorized into (1) spatial visualization, (2) spatial orientation, and (3) spatial relations (Bodner & Guay, 1997; Ferk et al., 2003). Spatial visualization describes an ability to understand accurately 3D objects from their 2D representations (Ferk et al., 2003). Therefore, it involves individuals mentally reconstructing or manipulating components of a visual stimulus and recognizing, retaining, and recalling configurations when the object is removed (Bodner & Guay, 1997, p. 6). Spatial orientation measures an ability to imagine what a representation will look like from a different direction. Spatial relations also involves an individual's abilities to mentally rotate, reflect, and inverse a mental configuration (Ferk et al., 2003).

Bodner and Guay (1997) summarized a review of literature on relationships between student performance on The Purdue Visualization of Rotations Test (ROT) and course exams. They suggested that the correlation between spatial ability and students' performance on chemistry exams was significant for questions that required students to mentally manipulate 2D representations of a molecule. However, the correlation between spatial ability and students' scores was not significant for questions that could be answered by rote memory or by applying a simple algorithm.

Ferk and colleagues (2003) indicated that the use of some types of 2D molecular representations will influence students' visualization. For example, about 96% of secondary chemistry students were able to construct 3D mental models based on a photograph of a concrete molecular model, yet only 74% of them succeeded on the basis of a stereochemical formula. Also, a student's correct perception of a 3D molecular structure is crucial for his or her mental operations (e.g., rotation, reflection, and rotation and reflection). Students' success decreased significantly when given a more complex molecule or when a combination of several mental processes were required (Ferk et al., 2003). This deficiency can hinder the students' understanding of stereochemistry, such as molecular shape, chirality, and stereoisomers (Briggs & Bodner, 2005; Stieff et al., 2005).

Summary

Review of research in this section shows that learning advanced or more abstract concepts requires a coherent conceptual framework consisting of prerequisite concepts. Missing prerequisite concepts or linkages among conceptions, partial or incorrect understanding, or fragmented conceptions may result in misconceptions or failure of learning. Most research on student chemistry conceptions at the submicroscopic-symbolic domain investigated students' knowledge and misconceptions in a limited content area, such as atoms and molecules (Cokelez & Dumon, 2005; Harrison & Treagust, 1996), ionization energy (Taber, 2003b), chemical bonding (Coll & Treagust, 2001; Jang, 2003), ionic bonding (Coll & Treagust, 2003a), covalent bonding, (Coll & Treagust, 2002; Peterson & Treagust, 1989; Peterson et al., 1989), metallic bonding (Coll & Treagust, 2003b), chemical reaction (Ben-Zvi et al., 1987; Hinton & Nakhleh, 1999), chemical equilibrium (Chiu et al., 2002; Kousathana & Tsaparlis, 2002), or molecular geometry and polarity (Furió & Calatayud, 1996; Furió et al., 2000).

For instructional purposes, it is important for chemistry instructors to understand how a sequence of concepts in their teaching influences learners' development of understanding, as well as to recognize essential concepts that bridge learners' understanding to the next level. Thus, there is a need for research to extend the area of investigation from examining students' knowledge about a single concept to their conceptual framework in order to reveal relationships between and among related concepts and its impact on student learning.

Common sense reasoning in chemical education is a relatively new. There were limited studies in this area. Major research on procedural difficulties (Furió & Calatayud, 1996; Furió et al., 2000; Kousathana & Tsaparlis, 2002) utilized multiple-choice, diagnostic instruments to reveal students' errors. Without examining students' thinking processes, attributing all student errors on functional fixedness and functional reduction could be over generalized. It is possible that students may make the same error in a multiple-choice question but for different reasons. Research on common sense reasoning needs to incorporate a qualitative approach by using a think-aloud technique to examine students' problem-solving processes.

Previous research that investigated students' conceptual framework focused on classifying their quality of knowledge as well as identification of misconceptions of different chemical concepts. Review of the literature on learning impediments for understanding chemical representation and models suggests that further research on student thinking needs to go beyond the idea of knowledge as propositional statements and start to explore relationships between representations and an individual's conceptual framework. How does prior knowledge and understanding about representations and models influence an individual's problem solving process? Does the problem solving process involve construction and use of mental models? Also, how do cognitive-computational demands, involving modeling ability, visual-spatial thinking, general reasoning, and chemisemiotics influence students' transition of understanding between submicroscopic level and symbolic level? These questions remain unanswered in the science education literature. Further research in this area is limited by a lack of theories developed to explain how students interpret the symbolic representations and connect it to their submicroscopic understanding. There is a need to incorporate these new aspects when studying student learning in chemistry. It is this need that provided the rationale for this study.

CHAPTER THREE

METHODOLOGY

This chapter presents research questions and hypothesis, context of the study, overall mixed-method design, and method of participant selection. Details about data collection and data analysis techniques for quantitative and qualitative phases will be addressed in the following subsections.

Research Plan

There are two things a researcher needs to consider when designing a study to investigate students' understanding of molecular polarity. First, the researcher must investigate individuals' understanding about prerequisite concepts to identify their conceptual framework about molecular polarity. Second, the researcher invents a way to diagnose learning obstacles and distinguish obstacles about visual-spatial thinking or construction of mental representations from a lack of prerequisite concepts or fragmental conceptual framework.

Considering the two ideas discussed above, this study employed a mixed-method design to examine undergraduate general chemistry students' understanding of molecular polarity. Taber (2000) argued that grounded theory provides a methodology which may build on strengths of both quantitative and qualitative research paradigms. He suggested researchers using quantitative diagnostic instruments to provide data of students' understanding about prerequisite concepts that feeds back into an emergent model from the qualitative data. The quantitative data will act both to triangulate the interpretation of the qualitative data, and increase the generality of aspects of the emergent model encompassing responses from a larger number of students.

Based upon Taber's (2000) suggestions, the quantitative part of this study adapted three instruments from the science education literature to diagnose characteristics and structures of conceptual frameworks that college students possess regarding molecular polarity. In addition, the diagnosed conceptual framework of interviewed participants served as a data source to triangulate findings from within-case analyses. The design and implementation of the qualitative part is guided by a theoretical framework of personal constructivism and a case study methodology. Through case study and grounded theory approach, the researcher provided a holistic view of college chemistry students' use of conceptual framework and mental models to solve problems about molecular polarity. In addition, this approach will provide possible explanations for what contributes to students' difficulties learning molecular polarity.

Research Questions and Null Hypotheses

This study was designed to investigate this overarching research question: What are the influences on students' problem-solving about molecular polarity? The following sub-questions were developed to answer the overarching research question from both quantitative and qualitative phases.

Quantitative:

1. Is there a difference between male and female general chemistry students on their course performances in terms of exams 1, 2, 3, final exam, and course grade?

   H_0^1 There is no significant difference between male and female students on their course performances in terms of exams 1, 2, 3, final exam, and course grade.

2. Is there a difference between male and female general chemistry students on their score of instrument EN regarding understanding of concepts about electronegativity?

H_0^2 There is no significant difference between male and female students on their score of instrument EN regarding their understanding of concepts about electronegativity learned by the general chemistry students.

3. Is there a difference between male and female general chemistry students on their score of instrument CB regarding understanding of concepts about chemical bonding?

   H_0^3 There is no significant difference between male and female students on their score of instrument CB regarding their understanding of concepts about chemical bonding learned by the general chemistry students.

4. Is there a difference between male and female general chemistry students on their score of instrument GP regarding understanding of concepts about molecular geometry and polarity?

   H_0^4 There is no significant difference between male and female students on their score of instrument GP regarding their understanding of concepts about molecular geometry and polarity learned by the general chemistry students.

5. What are the relationships between each exam and final score of this course and scores of the instruments EN, CB, and GP for the undergraduate general chemistry students?

   H_0^5 There is no significant correlation between participants' exams and final score of this course and their scores of the instruments EN, CB, and GP.

6. Is there a difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their course performances in terms of exams 1, 2, 3, final exam, and course grade?

H_0^6 There is no significant difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their course performances in terms of exams 1, 2, 3, final exam, and course grade.

7. Is there a difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their score of the instrument EN?

   H_0^7 There is no significant difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their score of the instrument EN.

8. Is there a difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their score of the instrument CB?

   H_0^8 There is no significant difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their score of the instrument CB.

9. Is there a difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their score of the instrument GP?

   H_0^9 There is no significant difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their score of the instrument GP.

10. What are the common misconceptions regarding molecular polarity and its prerequisite concepts (electronegativity, chemical bonding, and molecular geometry) for the undergraduate general chemistry students?

Qualitative:

11. What mental-modeling ability do high-scoring, moderate-scoring, and low-scoring students possess regarding molecular polarity?

12. What conceptual framework do high-scoring, moderate-scoring, and low-scoring students possess regarding molecular polarity? Specifically, describe the quality and

content of conceptual framework regarding molecular polarity possessed by high-scoring, moderate-scoring, and low-scoring students.

13. What mental models do high-scoring, moderate-scoring, and low-scoring students construct regarding molecular polarity? Specifically, describe the quality and content of mental models regarding molecular polarity possessed by high-scoring, moderate-scoring, and low-scoring students.
14. What contributes to the differences between high-scoring, moderate-scoring, and low-scoring students on their understanding of molecular polarity? Specifically, are they due to a lack of prerequisite knowledge and/or fragmental conceptual framework? Or are difficulties due to a lack of construction and utilization of mental models as tools of thinking? In this study, a theory was developed to explain how general chemistry students' conceptual framework and mental models influence their learning about molecular polarity.

Context of the Study

Course Structure

This study took place in a second course of a three-course general chemistry sequence (Chemistry 1310, 1320, and 1330) at a Midwest research extensive institute during the Fall 2006 semester. Students enrolled in Chemistry 1320 either had completed the first course of the general chemistry sequence (Chemistry 1310) with a prerequisite of grade of C- or better, or were considered having good high school background in chemistry and satisfied the campus College Algebra requirement (Undergraduate 2006-2008 Catalog Extracts: College of Art and Science, 2006). This course was also eligible as an honors course with extra coursework for honors-eligible students. Eleven students enrolled in the class for honor credits.

Table 3 lists content topics, based on the textbook *Chemistry* (Chang, 2005), that were the primary text for Chemistry 1320. The concept of molecular polarity was introduced in the second half of the semester. Prerequisite concepts and textbook chapters related to molecular polarity include (a) ionization energy (Chapter 8), (b) chemical bonding, electronegativity, and Lewis structure (Chapter 9), (c) molecular geometry, dipole moment, valance bond theory, and hybridization (Chapter 10), and (d) intermolecular force (Chapter 11).

Table 3

Class Schedule and Content Topics

Class schedule	Content topics
August 21	Chapter 6. Thermochemistry
September 4	Chapter 7. Quantum Theory and the Electronic Structure of Atoms
September 21	Exam I
September 25	Chapter 8. Periodic Relationships Among the Elements
October 9-15	Instrument EN was administrated
October 10	Chapter 9. Chemical Bonding I: Basic Concepts
October 16-23	Instrument CB was administrated
October 16	Chapter 10. Chemical Bonding II: Molecular Geometry and Hybridization of Atomic Orbitals
October 31-November 6	Instrument GP was administrated
November 2	Exam II
November 13	Chapter 11. Intermolecular Forces and Liquids and Solids
November 27	Chapter 12. Physical Properties of Solutions
December 6-7	Exam III and Final exam

Concepts Associated with Molecular Polarity

For studying learners' conceptions, researchers (Jang, 2003; Peterson et al., 1989; Tan & Treagust, 1999) have used concept webs to represent hierarchies of generalization by expressing propositional linkages within systems of related concepts. The structural features of the map allow researchers to define the boundary of content area and to organize related concepts based on their hierarchical relationships (Jang, 2003). In this study, a concept map for molecular polarity (Figure 4) was developed, and the components of the concepts were determined based on the text – *Chemistry* (Chang, 2005). The components and structure of the concept map were validated by a panel of experts including a chemistry faculty member and three science education faculty members.

Four major concepts emerged from the concept map of molecular polarity: (1) periodic variation (including atomic model and valence electrons), (2) chemical bonding (including construction of Lewis structure), (3) electronegativity and dipole moment, and (4) molecular geometry are considered essential for understanding molecular polarity. Intermolecular force and properties of liquids and solution process concepts were considered at a higher hierarchical level than molecular polarity.

The valence-shell electron pair repulsion (VSEPR) model is often used to predict the geometry of a molecule in the chemistry community. The VSEPR model assumes that electron pairs in the outermost electron shell (the valence shell) of an atom repel one another. In a molecule composed of multiple atoms, the central atom can be surrounded by two or more bonding pairs and lone pairs of electrons. Due to the repulsion between negative charges of the electron pairs, the bonding and lone pair electrons will remain as far apart as possible to minimize the repulsion. Applying this idea to a Lewis dot structure of a molecule and rearranging the electron pairs (including both bonding and lone pairs) spatially to be as far apart as possible, one can successfully predict the overall geometry of a molecule. An additional notion to the VSEPR model is that electrons of a

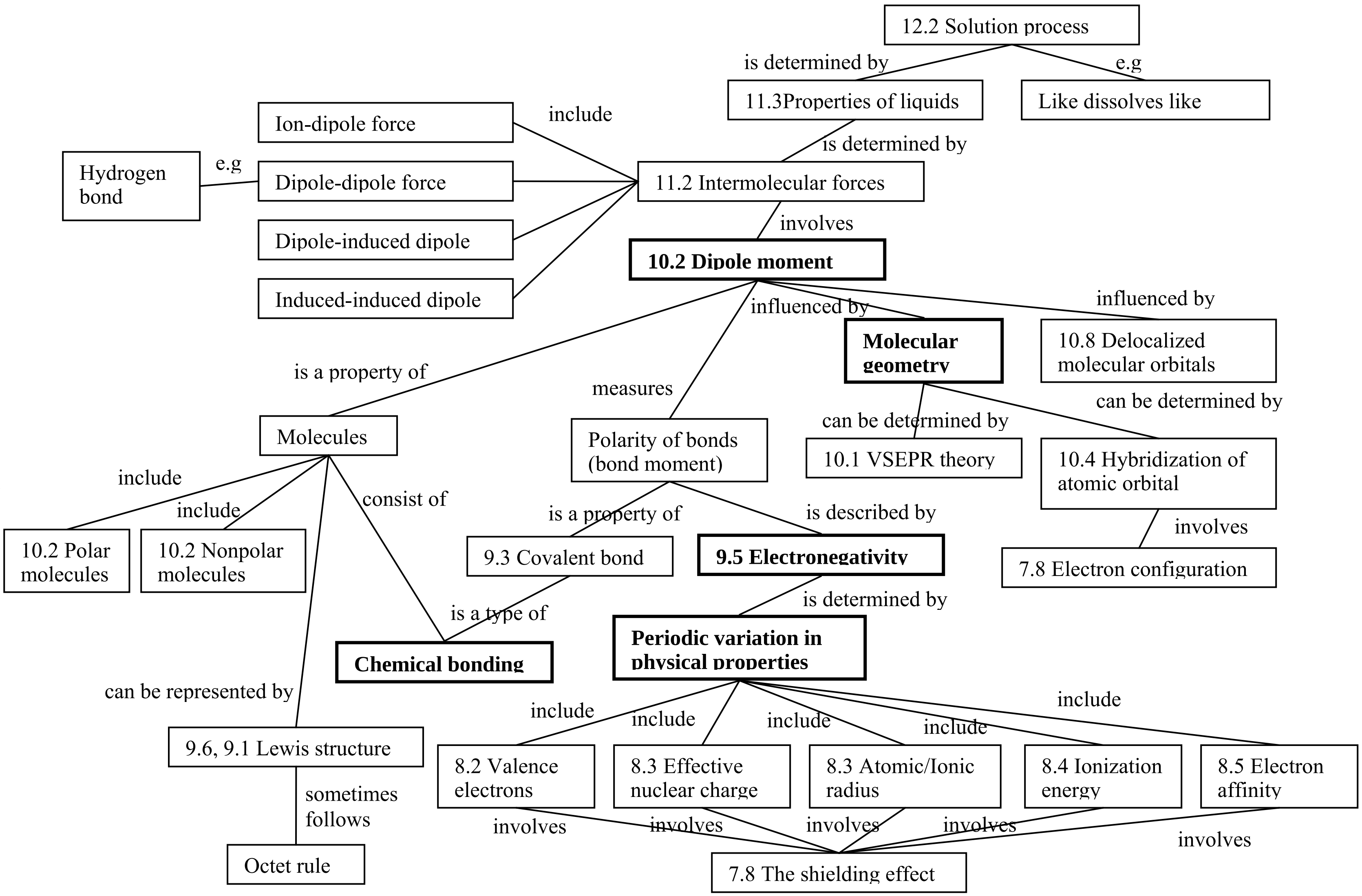


Figure 4. Concept map for molecular polarity (based on Chang, 2005).

bonding pair are held by the attractive forces exerted by the nuclei of the two bonded atoms. Electrons of a lone pair, which are associated with only one atom, exert greater repulsive force to the neighboring electron pairs; therefore, occupy greater space spatially compared with the bonding pairs (Chang, 2005).

Overall Design of the Study

To gather data for answering the research questions, this study used a two-phase design consisting of a quantitative approach in phase one and a qualitative approach in phase two.

For eliciting students' conceptual framework about molecular polarity, three diagnostic instruments were used to gather information about percentages of correct and incorrect responses and types of misconceptions related to electronegativity, chemical bonding, and molecular geometry and polarity. These three diagnostic instruments included: (1) a diagnostic instrument on electronegativity (instrument EN, see Appendix B) (Taber, 2002b), (2) a two-tier diagnostic instrument on chemical bonding (instrument CB, see Appendix C) by combining selected items from Peterson et al., (1989) and Jang (2003), and (3) a diagnostic instrument on molecular geometry and polarity (instrument GP, see Appendix D) (Furió et al., 2000; Peterson et al., 1989). Each instrument was administrated to the whole class as a concept exercise on BlackBoard after corresponding topics were introduced. Chemistry students could complete each instrument more than once; their final score was used for this study.

For the qualitative component of the study, a combination of think-aloud protocol and interview-about-events (White & Gunstone, 1992) was used to collect data of students' explanations and their constructions of artifacts (including drawings and model constructions). The multiple-case study allowed the investigation of participants' thought processes and descriptions of their cognitive activities holistically--organizing and applying existing knowledge, constructing mental models, and used both knowledge and mental models while solving molecular polarity problems. Grounded theory approach, employing a constant comparative method, allowed me to examine emergent patterns, themes, and categories within and across cases. In addition, this provided possible explanations of the relationships between participants' conceptual framework and mental models and to what attributes the variation of students' learning about molecular polarity. Figure 5 illustrates the process of data collection and data analysis in this study.

Quantitative Research Phase

The first phase of this study investigated students' conceptual framework about molecular polarity using the three diagnostic instruments. The instruments also allowed me purposeful sampling for case selection at phase two. The three diagnostic instruments were completed after students received instruction on the corresponding conceptions. Thus the researcher used the diagnostic instruments as post-instructional assessments to study outcomes of learning and did not manipulate the variables.

Variables

Independent variables of this study were gender (male and female) and number of chemistry courses participants enrolled (in high school and college levels) prior to Chemistry 1320 ($n = 0, 1, 2,$ and ≥ 3). Dependent variables are students' scores on instrument EN, instrument CB, and instrument GP, as well as scores of four course exams, and final course grade.

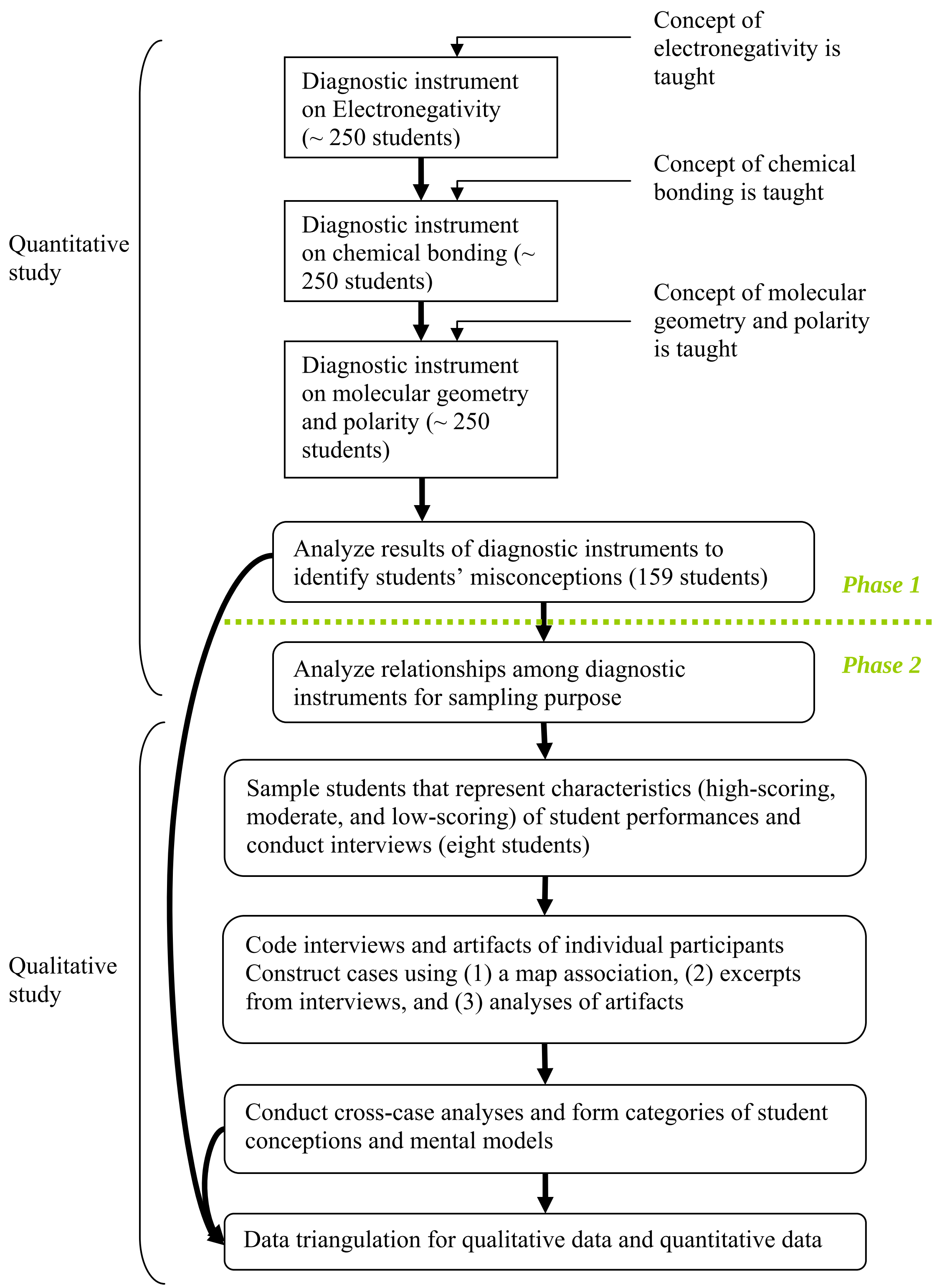


Figure 5. Process of data collection and analysis.

Instrumentation

To examine students' understanding of prerequisite concepts about molecular polarity, three diagnostic instruments (instruments EN, CB, and GP) were used to gather information about percentages of correct and incorrect responses and types of misconceptions related to electronegativity, chemical bonding, and molecular geometry and polarity. These three diagnostic instruments served three purposes:

a. To provide background information of commonalities between learners in terms of their level of understanding about molecular polarity and potential misconceptions. Taber (2000) suggested that data of diagnostic instruments provides data about ideas that students commonly hold in the classroom.
b. To serve as a sampling technique to select participants for the phase two interviews (the criteria of sampling is discussed in *Participants* section). This increases the generalizability of case studies to include other students who are not involved in the interviews (Taber, 2000).
c. To serve for data triangulation purpose. A participant's responses on the three diagnostic instruments provide information about his or her existing knowledge. The researcher is able to triangulate participants' conceptual understanding and alternative conceptions identified from the three instruments to the findings from interview analyses and interpretation.

Four instruments from science education literature were modified to fit the focus of this study. Items from the original instruments that did not directly address molecular polarity or its prerequisite concepts were deleted. Instruments EN, CB, and GP were finalized and used to assess students' understanding about electronegatibity, chemical bonding, and molecular geometry and polarity, respectively. Information about each instrument is described as following:

1. Instrument EN – *Chemical Misconceptions – Ionization Energy Probe* is a paper-and-pencil instrument comprised of 20 items of true/don't know/false questions (Taber, 2002b). It was a short version of the original 30-item version, developed by Taber (2000; 2002b; 2003b) to assess college students' understanding about ionization energy. This instrument was first administrated to 209 chemistry students at college level in the United Kingdom (UK) and verified with data of 15 student interviews (Taber, 2000). It was later administrated to over 300 college level chemistry students from 17 institutions in the UK (Taber, 2003), and the identified students' alternative conceptions in this large-scale study aligned with findings of the previous research (Taber, 2000). No validity and reliability was reported in these studies; however, the diagnosed misconceptions based on participants' interviews (Taber 2000) supported the results of the diagnostic instrument (Taber 2000; 2003). Concepts assessed by the *Ionization Energy Probe* included the concepts on electronegativity in Chemistry 1320. Therefore, the instrument was renamed to instrument EN to prevent students' confusions.
2. Instrument CB – A two-tier multiple choice diagnostic instrument, *Covalent Bonding and Structure*, was developed by Peterson et al. (1989) to investigate student understanding on covalent bonding and molecular structure. Items about molecular structure in Peterson et al.'s *Covalent Bonding and Structure* were selected to form instrument GP, and the remaining items were merged with selected items from Jang's (2003) *Chemical Bonding Diagnostic Test* regarding chemical bonding to form the

instrument CB. Peterson et al's and Jang's two-tier diagnostic instruments were administrated to Grade 11 and 12 chemistry students in Australia (total 243 students) and South Korea (total 816 students), respectively. Both Peterson et al.'s and Jang's instruments were tested for content and expert validation and had a Cronbach alpha reliability of 0.73 (15 items) and 0.74 (15 items), respectively.

3. Instrument GP – Furió et al.'s (2000) *Questionnaire 2* is an instrument consisting of 8 multiple-choice questions to assess students' understanding about molecular geometry and polarity. This instrument was administrated to 85 Grade 12 chemistry students, 151 first-year and 100 third-year undergraduate students in Spain. No validity and reliability was reported in Furió et al.'s study. Two-tier items in Peterson et al.'s *Covalent Bonding and Structure* regarding molecular structure were merged with items in Furió et al.'s (2000) *Questionnaire 2* to form the instrument GP. Instruments EN, CB, and GP are in Appendix B, C, and D, respectively.

Participants

A majority of students in Chemistry 1320 were freshmen. After an introduction to this study, students were encouraged to participate at one or two levels, and signed a consent form (see Appendix A). This study (project number--1076257) was approved by University of Missouri-Columbia (MU) Campus Institutional Review Board (IRB) prior to any data collection procedure. Under the guideline of MU Campus IRB, only students who gave permission to access their responses and scores were included as participants of the study. Whether or not the students participated in the study did not influence their course grades. Among approximately 250 students in the class, 159 students granted access to the researcher to use their responses and scores for phase one analysis with 48 who volunteered for interviews.

Data Collection

Each diagnostic instrument was given as a supplemental concept exercise on an electronic education system – the BlackBoard system after the instruction of the corresponding textbook chapter. Instruments EN, CB, and GP were given as concept exercises of Chapter 7–Quantum Theory and the Electronic Structure of Atoms, Chapter 9–Chemical Bonding I: Basic Concepts, and Chapter 10–Chemical Bonding II: Molecular Geometry and Hybridization of Atomic Orbitals, respectively (see Table 3). Students were encouraged to complete the concept exercises to provide feedback for improving course instructions. The BlackBoard system provided feedback as "correct" or "incorrect" when students responded to each item.

Items of each diagnostic instrument were scored electronically on the BlackBoard system. For the two-tier test items, answers were considered correct if the student was correct in both content and reasoning questions. Both correct and incorrect responses of items in the instruments EN, CB, and GP were calculated. The total points for instruments EN, CB, and GP are 20 points, 7 points, and 15 points, respectively. Analysis of incorrect response combinations provided data on students' misconceptions of concepts and propositions related to that item.

Reliability analysis. Internal consistency is an indicator of how well different items measure the same concept. Generally, reliability coefficients of 0.70 or more are considered good (Vogt, 2007). Internal consistency reliability for instruments EN, CB, and GP was calculated for the 159 participants. The reliability coefficients (Cronbach's alpha) for instruments EN (20 items), CB (7 items), and GP (15 items) were 0.49, 0.55, and 0.76, respectively.

Statistical analysis of data. According to Taber (Taber, 2000, 2003b), instrument EN elicited three alternative frameworks associated with electronegativity: (1) orthodox electrostatics, refers to the evidence that students do not apply Coulombic principles to nucleus-electron interactions (item 2, 5, 6, 8, 11, 13, 14, 16); (2) an alternative electrostatic principle – conservation of force, refers to the conception that the nuclear charge exerted from an atom's protons is in some sense shared out amongst the electrons (items 15, 17, 19); and (3) an alternative notion of stability – octet rule framework, refers to that an atom would not be considered stable as it does not have a full outer shell (items 1, 3, 4, 12, 18, 20). Instruments CB and GP were used to determine students' misconceptions about (1) octet rule, (2) covalent bonding, (3) ionic bonding, (4) bond polarity, (5) molecular shape, (6) polarity of molecules, and (7) intermolecular force (Furió et al., 2000; Jang, 2003; Peterson et al., 1989). Items associated with diagnosing specific misconceptions were combined, and percentages of students possessing specific misconceptions or alternative framework were calculated to compare with the findings from literature for answering research question ten.

Descriptive statistics and two one-way analysis of variance (ANOVA) were performed to analyze the relationships between gender (research question one, two, three, and four), as well as the number of chemistry courses participants enrolled prior to Chemistry 1320 (n = 0, 1, 2, and $\geq$ 3) (research question six, seven, eight, and nine) and their scores of the instruments EN, CB, and GP; and Pearson's correlation coefficients (r)

were calculated to examine research question five. An alpha level of .05 was used for all statistical tests.

Qualitative Research Phase

Research Tradition

The second phase of the study focused upon an individual's thinking process while solving molecular polarity problems, specifically, examining whether the individual constructs a physical or mental model based on his or her existing knowledge, and whether the individual uses the model as a tool of thinking. If a mental model is constructed, what does it looks like? Is it static or dynamic? How does the individual manipulate the physical or mental model? To what extent is the individual's mental model related to his or her conceptual framework? How does the individual use the conceptual framework and mental model to seek for the solution path? Moreover, how does the quality and structure of the conceptual framework and mental models influence the individual's successfulness and unsuccessfulness of problem solving?

Because of my interest in the process of sense-making and mental model construction in one's mind, I adopted a personal constructivist lens with an integration of Briggs's (2007) Models and Modeling theoretical framework. Constructivists believe that an individual applies existing knowledge to make sense of a new concept and incorporate that into the existing knowledge (Ferguson, 2007). Briggs said that "a real world exists outside of one's mind … and one can never know the true nature of something because one always views the thing through the filter of senses and experience" (p.73). Due to knowledge, experience, and reasoning varying among individuals, the truth and reality that one believes is relative (Ferguson, 2007; Patton, 2002). Therefore, each case stands as a unique case to inquire.

My epistemological assumption of this study is that knowledge is never transmitted directly from the instructor to the learners (Ferguson, 2007). Instead, an individual actively constructs knowledge through examining new information in their existing knowledge and experience. In addition, the learner "invents concepts and models to make sense of the incoming information and then continually tests and modifies these constructions in the light of new experiences" (Briggs, 2007, p. 13). Therefore, the constructed new concept and model is strongly associated with and needs to be interpreted within the individual's overall structure of existing knowledge.

Using conceptual change theories (Chi, 1992; Mortimer, 1995), another epistemological assumption is the possibility of an individual possessing a manifold of conceptions (in Chi's words, different ontological perspectives, or Mortimer described it as conceptual profiles) and applying a specific conception according to the context of a problem (Mortimer, 1995). An individual may also construct various mental models for the same concept, which explains how students may possess alternative and scientific conceptions simultaneously but applies them in different contexts (Briggs, 2007). This ability to construct multiple systems of representations for the same concept varies among individuals.

A case study employing a hermeneutical cycle that allowed me to see a participant's sense-making or meaning-making experience from a personal perspective by interpreting the dialogues and artifact productions in his or her global meaning of a specific concept (Patton, 2002). Explanations that students offered provided information about how students organized, related, and integrated chemistry concepts and principles to a specific model in chemistry (O'Connor, 1997). Therefore, I believe that an individual's understanding of molecular polarity can be studied by constructing a case using multiple data sources: (1) quality and structure of the prerequisite knowledge gathered through diagnostic instruments, (2) artifacts such as drawings and model construction, and (3) dialogues about their processes of reasoning using conceptual framework and physical and/or mental representations to solve problems during interviews (Briggs, 2004; Patton, 2002).

Creating multiple cases through purposeful sampling based on responses to quantitative instruments allowed the study to address the question: What are the differences between students who are successful and unsuccessful at solving molecular polarity problems? Semi-structured interview protocols (Appendix E) guided each participant as they worked through the same set of thought-revealing tasks; thereby, providing a base to compare thinking processes within and across cases. At the same time, they allowed me to probe into the ideas that are unique to the individuals.

Within the science education literature, there is no reported research to describe the interaction between an individual's conceptual framework and his or her construction and use of mental models. Grounded theory approach provides a possible avenue to create new and theoretically expressed understandings, where "theory was strictly derived from data, systematically generated and analyzed through the research process" (Strauss & Corbin, 1998, p. 12). The coding procedure of the grounded theory gives an analytic tool for categorizing data of multiple cases and a comparative method to examine patterns, themes, and categories within and across cases to form a model or theory.

Role of the Researcher

Lincoln and Guba (1985) emphasized the importance of building and maintaining trust for qualitative research. Participants need to feel comfortable to talk with the researcher to express their ideas. To create a trust relationship, I contacted all the participants on a one-to-one basis to carefully explain my research goals and activities to develop the trust among myself and the participants prior to the interview. Participants viewed me as a graduate student in science education who wanted to study their thinking processes and learning difficulties to improve future college chemical instruction. Thus, they were open to conversations with me and tried to make their thinking processes explicit to help data collection. They also trusted me as a chemistry expert who would identify their misconceptions during the interview and provide feedback to them at the end of the interview as a mini-tutor section. However, three students felt uncomfortable about the interview and were nervous about giving wrong answers. Therefore, their expressions about conceptual framework, mental models, and reasoning processes were highly influenced within this situation. All three of these students were categorized as low-scoring students based on their responses to instruments EN, CB, and GP. Therefore, I assumed that their anxiety about the interview process may have resulted from their low confidence about chemical understanding.

During the interview, I probed and inquired into the participant's thinking processes through interactive dialogue with the participant (Coll & Taylor, 2001). My chemistry background allowed me to identify participants' misconceptions and the quality and accuracy of their explanations during the interview. I was able to use probing questions to elicit the presuppositions behind their answers, to interpret their use of language, and to diagnose the generated models when participants described a chemical phenomenon.

I was aware that the revealed conceptions and mental representations were influenced by the interactions between the participants and me (Coll & Taylor, 2001). My understanding of chemistry concepts, ontological and epistemological beliefs, and interactions with a participant in the previous interview may become my biases. It was not possible to be completely free of bias when I probed during interviews or when analyzing and interpreting data.

Data Collection

Research in conceptual change (Hewson, 1981, 1996; Posner et al., 1982; She, 2004; Vosniadou, 1994, 2003) indicated that individuals possess conceptual frameworks and construct mental models about a specific concept that is unique to the individuals who construct them. To elicit the unique cognitive activities of each individual, I developed an interview protocol (Appendix E) consisting of thought-revealing tasks based on the guidelines suggested by Briggs (2007). The interview protocol was developed based on literature of diagnosing student misconceptions about atoms and molecules (Taber, 2002a) and chemical bonding (Nicoll, 2001). Interview questions started by focusing on fundamental concepts, such as atomic model and valance electrons (Q1), bonding (Q2), then gradually shifted to higher hierarchical concepts like molecular geometry and polarity (Q6, 7, and 8). These interview questions were designed to reveal both participants' application of existing knowledge as well as their construction and use of mental models. Thus, I specifically probed for meaning when participants used a specific term and what concepts they associated with each question. I asked the participants constantly for whether or not they used a mental image while thinking through the tasks, and probed for details about features of the mental model and actions of applying these models by encouraging them to draw, describe, and build models with play-dough and straws.

To reduce the likelihood of misinterpretation, I used pairs of questions to probe the same concept with different examples for data triangulation. For instance, in addition to asking “What does the term ‘polar molecule’ mean to you”, interview question 6 and 7 used H_2S (a polar molecule) and BF_3 (a non-polar molecule) to probe participants’ ideas about molecular polarity. Questions 2, 5, 8, and 9 were designed to elicit mental models in actions. These questions required participants to be conscious about their mental model (if they constructed one) and to assess their ability to manipulate the mental model to answer the questions.

Three molecules--hydrogen sulfide (H_2S), sulfur dichloride (SCl_2), and boron trifluoride (BF_3), were used for interviews to elicit students’ thinking processes about molecular shape and polarity. The molecular structure of BF_3 was discussed in the lecture and the textbook as a trigonal planar shape. The H_2S and SCl_2 molecules were not mentioned in the textbook. However, the water (H_2O) molecule, that has a similar structure with H_2S and SCl_2, was discussed in the class. H_2O, H_2S, and SCl_2 molecules all have a bent molecular shape, and their arrangement of the four electron pairs is tetrahedral.

H_2S represents a polar molecule which consists of two lone pair of electrons and two bonding electron pairs that each bonds to a hydrogen atom. The purpose of using H_2S molecule was to elicit students’ perceptions about (1) lone pairs, (2) preferred chemical representations while working on a problem, (3) arrangement of electron pairs (including two bonding and two lone pairs) in three dimensions, (4) bond angles, and (5) their thinking processes while considering factors that influence the molecular shape and polarity. Considering the VSEPR model, the result of a bond angle comparison for SCl_2, H_2S, and a molecule with a right tetrahedral shape (e.g. CCl_4) is $SCl_2 < H_2S < CCl_4 = 109.5°$.

BF_3 represents a nonpolar molecule in a trigonal planar shape. It is also an exception of the octet rule without lone pairs present. According to the VSEPR model, each of the three FBF angles is 120°, and all four atoms lie in the same plane. BF_3 allowed me to investigate students' responses to an exception of the octet rule and their perceptions about a trigonal planar molecule. Comparing students' thinking processes while solving problems related to BF_3 and H_2S provided an opportunity to examine the stability of participants' approaches to determine molecular shape and polarity.

Interview implementation. All interviews were scheduled at the end of the fall semester, 2006. For students who were interviewed ($n = 8$), each interview was approximately 1 hour in length. One video camera was used near the ceiling to record the student's drawing and model constructions as they were generated in real time.

Participants were given a short description about the purpose of the interview, to study how chemistry students conceptualize concepts of atoms, molecules, and polarity and whether they use physical or mental representations to facilitate their thinking processes when solving chemical problems. They were assured verbally that this study was independent of their classroom assessment and that their responses would not be identified to the instructor. Students were told that they would be asked to monitor and be explicit their thinking processes, and their detailed, explicit elaborations on interview responses were greatly valued. To encourage participants to express their entire thinking processes during the interview rather than only the correct answers, I explained to the students that the textbook answers to the interview questions would be discussed at the end of the interviews as a mini-tutor section.

Interviews started with eliciting a participant's ideas about atomic structure, periodic trends, and procedures to derive a Lewis structure from a chemical formula. Participants were then asked to build a model to represent geometry of the molecule from the Lewis structure, followed by questions prompting him or her to describe features of the model including chemical bonds, shape of lone pair electrons, electron distributions, and interactions (e.g., attraction or repulsion) among bonding and bonding electron pairs. Students were then asked to determine polarity of the molecule.

Meanwhile, each participant was prompted frequently to consciously monitor their thinking processes or strategies, for example, generating mental images, memorizing definitions and statements, or using routines of problem solving strategies in his or her mind. In addition, the participant was encouraged to draw on paper or build models using play-dough and straws to describe their mental images to the researcher. Throughout the interview, the participant was permitted access to the Periodic Table and a textbook since this research focused on how students used representations and models to facilitate their reasoning of problems regarding molecular polarity.

All data in this study on students' mental models and reasoning included their responses to three online diagnostic instruments, student-generated diagrams and models, and verbal explanations accompany their diagrams and models. Appendix F illustrates the correspondences between research questions and sources of data collection.

Data Analysis

The primary data sources were video-taped interviews and artifacts, such as drawings or models that participants generated during the interviews. Participants' responses to three diagnostic instruments at phase one of the study served as a secondary data source. I transcribed all eight video-taped interviews verbatim and then reviewed each interview transcript for accuracy. I categorized interview participants into high-, moderate-, and low-scoring groups based on their percentages of questions answered correctly on three diagnostic instruments. Table 4 lists the categories and the eight participants' numbers of correct items on the diagnostic instruments:

Table 4

Categorization of Interview Participants Based on Their Numbers of Correct Items on Instruments EN, CN, and GP

	Participants (rank based on numbers of correct items)	Instrument EN (Total: 20 items)	Instrument CB (Total: 14 items)	Instrument GP (Total: 26 items)
High-scoring students	JS (h, h, h)	16	11	20
	CR (m, h, h)	11	13	23
	RE (l, h, h)	10	13	23
Moderate-scoring students	TA (l, m, m)	7	9	18
	SD (l, m, m)	5	9	15
Low-scoring students	KA (l, l, n/a)	7	6	n/a
	AM (l, l, l)	4	5	13
	JT (l, m, l)	10	9	9

The next step was to code the videos to identify participants' conceptual frameworks and mental models about molecular geometry and polarity and the prerequisite concepts.

Analyses of participants' conceptual frameworks. I applied an open coding process to the interview videos to categorize a participant's explanations considering both verbal and nonverbal (e.g. hand gestures, drawing, and construction of models) data as expressed explanations. The development of concept webs was grounded in interview data. To analyze participants' conceptual framework, I used a high-scoring student's conceptual framework as a criterion for cross-cases analyses, instead of comparing students' conceptual framework to a content authority, such as the textbook or the class instructor. I started coding the videos with three high-scoring students for key concepts and subsequent concepts about atomic model, chemical bonding, and molecular geometry, polarity, and electron-cloud model.

I developed codes as elements of a conceptual framework and connected these elements with links based on participants' verbal and nonverbal explanations. I combined some elements into a more representative concept and modified some links by testing elements and compared the links of concept webs for JS, RE, and CR against each other. Three initial concept webs about atomic model, chemical bonding, and molecular geometry, polarity, and electron-cloud model resulted from this coding process. I applied these three initial webs to analyze videos of moderate- and low-scoring students and then revisited high-scoring students' videos. The reviewing and recoding processes were repeated until the generated elements and links of the concept webs were saturated.

Ten clusters of key concepts and subsequent sub-concepts were identified and organized in these three concept webs. These clusters of concepts are listed in Table 5.

Table 5

Key Concepts in the Three Concept Webs that Represent a Participant's Conceptual Frameworks

Concept webs	Key concepts
Atomic model	I. Structure of an atom
	II. Periodic trend
	III. Atomic models
Chemical bonding	IV. Coulombic principle
	V. The octet rule
	VI. Chemical bonding
Molecular geometry, polarity, and electron-cloud model	VII. Molecular shape
	VIII. The VSEPR model
	IX. Molecular polarity
	X. Electron-cloud model

I recoded each interview in order to verify or modify the elements and links to the initial webs to best represent the participant's conceptual frameworks. Participants' construction and use of representations, meanings of these representations to the participant, and patterns of reasoning were also analyzed to add features to their quality of understanding.

Meanwhile, the three concept webs were recoded to portray each participant's quality of understanding. I examined each element and link against the participant's explanations and modified the elements and links to represent: (a) correct conceptions (ovals with solid line), missing conceptions (ovals with broken line), or misconceptions (ovals with bold line), as well as (b) correct links (solid lines), missing links (broken lines), or wrong connections (bold lines) between concepts. I used precise vs. vague and accurate vs. partially accurate to indicate correct conceptions if enough information was provided in students' explanations (White & Gunstone, 1992).

Types of elements were another feature of conceptual frameworks revealed from the coding processes. Types of information that students associated with a specific concept include propositions, rules or algorithm, 2D image, 3D mental image, episode, and personal theory. Among these types of information, rules represented steps or procedures that students follow without understanding appropriate explanations behind them. Episodes described information that a student visualized as an animation or a scene having objects with motions. For example, when RE described metallic bonding, she said, "all the nucleuses" with her hand gestures indicating imaginary nuclei arranged on the table; and when she continued: "with all the electrons just shared between all of the nucleuses" (RE, interview), her hands were waving on the imaginary nuclei to show movement of electrons among the nuclei as metallic bonds. Sometimes students generated an idea or a set of explanations about a concept that was theory-like, but differed from the scientific explanation. This theory-like explanation was labeled as personal theory.

Individual participant's responses to the three diagnostic instruments in the first phase of study were included to triangulate the mapping of conceptual frameworks. Strauss and Corbin (1998) suggested researchers consider the interplay between qualitative and quantitative methods to inform the emergence of a theory.

Next, I compared each case and performed axial coding (Strauss & Corbin, 1998) to look for similarities and differences between and among participants' conceptual frameworks. Three categories--high-, moderate-, and low-concept knowledge--emerged based on patterns and themes revealed from the cross-case analyses about characteristics of participants' conceptual frameworks. I then re-categorized the eight participants into these three categories and developed descriptions of students' conceptual understanding about molecular geometry and polarity and prerequisite concepts. The re-categorization reclassified TA from moderate-scoring group to low content knowledge group and moved AM from low scoring group to moderate content knowledge group.

For the analyses of mental models and mental modeling ability, I repeated the same analysis steps with the interview videos to analyze participants' mental models. I coded participants' verbal explanations and nonverbal data to look for features of individual's mental models and their cognitive moves related to construction and use of mental models during the problem-solving process. During the coding process, I developed categories and subcategories for features of participants' mental models and their mental-modeling ability. Then I elaborated each category and subcategory into a short descriptive sentence and organized them into two protocols, one for mental-modeling ability and the other for mental models.

A protocol of mental-modeling ability was composed of categories that described an individual's cognitive moves, excluding effects from the individual's content knowledge. A protocol of mental models included categories that described spatial and static features of participants' mental models in three dimensions as well as causal and dynamic features when the participants manipulated and/or used these mental models to solve a problem. I reviewed and recoded the videos several rounds until the categories were saturated.

Based on observations from the video analyses, each category in both protocols was assigned a score to reflect the relative degree that the category affected or depended on participants' thinking processes. Then I reviewed the videos and applied the protocols one at a time to score each interview. Again, I revisited and adjusted scores of some videos for several rounds until all the videos were scored appropriately.

For the protocol of mental-modeling ability, again, I compared each case and performed axial coding to explain similarities and differences between and among participants' mental modeling ability. Three levels--high-, moderate-, and low-mental modeling ability--emerged based on themes revealed from the within-case analyses. The eight participants were re-categorized into these three groups, and I developed descriptions of students' mental-modeling ability.

Based on results of categorization for level of content knowledge and mental-modeling ability, these eight interview participants were placed into a matrix to demonstrate an interaction between an individual's content knowledge and his or her mental-modeling ability. Each participant's score for the protocol of mental models was placed into the matrix to exemplify the results of the interaction.

Trustworthiness

Data triangulation has been addressed in two ways including the integration of quantitative and qualitative data and the use of multiple interview questions to study one concept. In addition, to ensure I used the same language and meaning of chemistry terminology with interview participants, I attended each related lecture to understand the instructor's approaches on introducing specific concepts. I especially paid close attention to the diagrams, animations, or models that may have influenced participants' construction and used mental models during interviews. The video-taped interviews also provided an opportunity for referential adequacy. The videos captured the episodes of the interviews that could later be reexamined and tested for adequacy for future critiques.

For transferability, I provided thick description about context, students' concepts and missing concepts, verbal and nonverbal expressions, and interactions between students and the interviewers to give a detailed description of the process as a whole. The thick description will help readers to understand how the findings are transferable to other situations.

Summary

This chapter presented research questions and hypotheses, the context, and the overall mixed-method design of the study. This study utilized three diagnostic instruments (instruments EN, CB, and GP) to elicit students' understanding and misconceptions about concepts of molecular geometry, polarity, and prerequisite concepts. Scores of the three diagnostic instruments were used to select eight participants for interviews. A grounded theory approach, employing a constant comparative method, was used to analyze the eight interviews. This analysis explored possible explanations on the relationships between participants' conceptual frameworks and mental models, as well as what attributes to the variation of students' learning about molecular polarity. I also described the methods of participant selection, data collection, and data analyses for both quantitative and qualitative phases of the study.

CHAPTER FOUR

FINDINGS

Introduction

This chapter is divided into two sections presenting findings of quantitative and qualitative phases. Findings for the quantitative phase include (1) results of descriptive and inferential statistical analysis, (2) results of individual instruments and diagnosed misconceptions, and (3) tests of the hypotheses. Findings for the qualitative phase about general chemistry students' conceptual frameworks and mental models are organized into three sections. I begin with a discussion of characteristics of students' mental-modeling ability. In the second section, I examine students' level of content knowledge by analyzing the content and quality of their conceptual frameworks. The final section addresses the interaction between participants' level of content knowledge and mental-modeling ability. Features of the participants' mental models were analyzed as outcomes of the interaction.

Quantitative Phase

Descriptive Statistics

Table 6 summarized total participants' means and standard deviations for scores on instruments EN, CB, GP, exams 1, 2, 3, final exam, and course grade by gender. The participants have a mean of 9.16 with a standard deviation of 2.88 for instrument EN. The mean and the standard deviation for instrument EN were 9.79 and 2.60 for male students, and 8.37 and 3.04 for female students, respectively. The mean and standard deviation of instrument CB were 3.58 and 1.51, respectively. The mean and the standard deviation for instrument CB were 3.61 and 1.63 for male students, and 3.54 and 1.39 for

Table 6

Mean and Standard Deviation of Scores on Instruments EN, CB, and GP by Gender

Instrument		*n*	*M*	*SD*
EN				
	Male	75	9.79	2.60
	Female	60	8.37	3.04
	Total	135	9.16	2.88
CB				
	Male	70	3.61	1.63
	Female	61	3.54	1.39
	Total	131	3.58	1.51
GP				
	Male	57	6.32	4.00
	Female	54	6.72	2.51
	Total	111	6.51	3.35

female students, respectively. Instrument GP had a mean and a standard deviation of 6.51 and 3.35, respectively. The mean and the standard deviation for instrument GP were 6.32 and 4.00 for male students, and 6.27 and 2.51 for female students.

The means and standard deviations of total participants' scores on exams 1, 2, 3, and final exam, and course grade were also calculated as 76.22 (*SD* = 13.84), 77.39 (*SD* = 14.11), 70.46 (*SD* = 15.43), 77.71 (*SD* = 12.40), and 81.38 (*SD* = 9.32), respectively (Table 7). The mean and the standard deviation of scores on exam 1 for male and female students were 76.46 (*SD* = 14.42), and 75.94 (*SD* = 13.21), respectively. The mean and the standard deviation for scores on exam 2 for male and female students were 77.85 (*SD* = 14.00), and 76.83 (*SD* = 14.35), respectively. The mean and the standard deviation of scores on exam 3 for male and female students were 72.28 (*SD* = 16.39), and 68.17 (*SD* = 13.95), respectively. The mean and the standard deviation for scores on final exam for male and female students were 78.77 (*SD* = 11.80), and 76.38 (*SD* = 13.08), respectively.

Table 7

Mean and Standard Deviation of Scores on Exams 1, 2, 3, Final Exam, and Course Grade by Gender

		n	*M* (%)	*SD*
Exam 1[1]				
	Male	79	76.46	14.42
	Female	64	75.94	13.21
	Total	143	76.22	13.84
Exam 2[1]				
	Male	79	77.85	14.00
	Female	63	76.83	14.35
	Total	142	77.39	14.11
Exam 3[1]				
	Male	79	72.28	16.39
	Female	63	68.17	13.95
	Total	142	70.46	15.43
Final Exam[1]				
	Male	79	78.77	11.80
	Female	63	76.38	13.08
	Total	142	77.71	12.40
Course Grade[1]				
	Male	79	81.75	9.46
	Female	63	80.91	9.21
	Total	142	81.38	9.32

[1]: Scores for exams 1, 2, and 3, final exam, and course grade are calculated in percentage

The mean and the standard deviation of scores on course grade for male and female students were 81.75 (*SD* = 9.46), and 80.91 (*SD* = 9.21), respectively.

Participants were also categorized based upon the number of chemistry courses they completed prior to the study. Only one individual had not enrolled in any previous chemistry course, and 45.7% (*n* = 58) of the participants had one chemistry course previously. Forty-four percent (*n* = 56) of the participants had two chemistry courses while 9.4% (*n* = 12) indicated that they had three or more chemistry courses prior to the study. Participants' scores of exams 1, 2, 3, final exam, and course grade were calculated in percentages. The means and standard deviations for the percentages of scores for exams 1, 2, 3, final exam, and course grade were then calculated based upon the number of previous chemistry courses (Table 8). The means and standard deviation of participants' scores on instruments EN, CB, and GP based upon the number of previous chemistry courses are presented in Table 9.

Table 8

Mean and Standard Deviation of Scores on Exams 1, 2, 3, Final Exam, and Course Grade by the Number of Previous Chemistry Courses

	Number of previous chemistry courses			
	0 (*n* = 1)	1 (*n* = 58)	2 (*n* = 56)	≥ 3 (*n* = 12)
	Score	*M* (*SD*)	*M* (*SD*)	*M* (*SD*)
Exam 1	40.00	76.47 (13.80)	77.28 (14.05)	79.17 (11.84)
Exam 2	60.00	78.79 (14.40)	79.11 (12.83)	83.33 (10.08)
Exam 3	55.00	70.52 (13.69)	72.86 (16.15)	74.58 (16.30)
Final Exam	69.00	78.38 (12.85)	77.61 (13.18)	79.92 (10.89)
Course Grade	68.70	81.91 (9.56)	82.10 (9.47)	83.68 (9.61)

[1]: Scores for exams 1, 2, and 3, final exam, and course grade are calculated in percentage.

[2]: The student's scores were reported for number of previous chemistry courses = 0 (*n* = 1).

Table 9

Mean and Standard Deviation of Scores on Instruments EN, CB, and GP by the Number of Previous Chemistry Courses

	Number of previous chemistry courses							
		0		1		2		≥ 3
	n	*Score*	*n*	*M* (*SD*)	*n*	*M* (*SD*)	*n*	*M* (*SD*)
Instrument EN	1	9.00	55	9.15 (2.93)	56	8.96 (2.97)	11	8.82 (2.96)
Instrument CB	1	1.00	54	3.59 (1.62)	54	3.69 (1.40)	11	4.00 (1.18)
Instrument GP	1	4.00	45	7.07 (3.19)	46	6.39 (3.21)	12	7.17 (3.56)

[1]: The student's scores were reported for number of previous chemistry courses = 0 (*n* = 1).

Analysis of Individual Instruments

Instrument EN

Participants' responses to items in instrument EN are indicated in Table 10. The percentage of students answering "don't know" ranges from 0% (item 1) to 12% (item 19). Items in instrument EN were grouped based on categories of conceptions that the original test items were designed to elicit (Taber, 2003). Evidence of students' misconceptions was established by students choosing a set of incorrect items. Items in both Tables 11 and 12 were sequenced based on percentages of incorrect responses. These categories include an alternative notion of stability (items 18, 20, 12, 4, 3, 1), an alternative electrostatic principle – conservation of force (items 17, 19, 15), and applying Coulombic principle (items 14, 6, 16, 13, 8, 5) (Table 11). Responses for a set of items designed to identify students' understanding regarding ionization energy were also analyzed (items 17, 11, 7, 9, 10, 2) (Table 12). The following subsections discuss students' alternative conceptual framework identified by clustered items of instrument EN with percentage incorrect for selected items.

An alternative notion of stability. Students' incorrect responses to items "the atom would be more stable if it 'lost' an electron" (92.0%, item 18), "the atom would become stable if it either lost one electron or gained seven electrons" (80.0%, item 20), and "if the outermost electron is removed from the atom it will not return because there will be a stable electronic configuration" (76.7%, item 12) reflected the participants' notion of "stability" and were closely associated with ideas of octet configurations, or full shells (Taber, 2003). In contrast to this alternative notion of stability, only 10% of the participants rejected the idea that "energy is required to remove an electron from the

Table 10

Responses to the Instrument EN (n = 150)

	TRUE *n* (%)	Don't know *n* (%)	FALSE *n* (%)
1. Energy is required to remove an electron from the atom.	135 (90.0%)*	0 (0.0%)	15 (10.0%)
2. After the atom is ionized, it then requires more energy to remove a second electron because the second electron is nearer the nucleus.	119 (79.3%)*	4 (2.7%)	27 (18.0%)
3. The atom will spontaneously lose an electron to become stable.	48 (32.2%)	5 (3.4%)	96 (64.4%)*
4. Only one electron can be removed from the atom, as it then has a stable electronic configuration.	89 (59.3%)	1 (0.7%)	60 (40.0%)*
5. The nucleus is not attracted to the electrons.	30 (20.0%)	4 (2.7%)	116 (77.3%)*
6. Each proton in the nucleus attracts one electron.	82 (54.7%)	7 (4.7%)	61 (40.7%)*
7. After the atom is ionized, it then requires more energy to remove a second electron because the second electron experiences less shielding from the nucleus.	61 (40.7%)*	13 (8.7%)	76 (50.7%)
8. The nucleus is attracted towards the outermost electron less than it is attracted towards the other electrons.	103 (69.6%)*	6 (4.1%)	39 (26.4%)
9. After the atom is ionized, it then requires more energy to remove a second electron because the second electron is in a lower energy level.	74 (49.3%)*	7 (4.7%)	69 (46.0%)
10. After the atom is ionized, it then requires more energy to remove a second electron because it experiences a greater core charge than the first.	105 (70.0%)*	17 (11.3%)	28 (18.7%)
11. After the atom is ionized, it then requires more energy to remove a second electron because it would be removed from a positive species.	45 (30.0%)*	17 (11.3%)	88 (58.7%)
12. If the outermost electron is removed from the atom it will not return because there will be a stable electronic configuration.	115 (76.7%)	4 (2.7%)	31 (20.7%)*
13. The force on an innermost electron from the nucleus is equal to the force on the nucleus from an innermost electron.	79 (52.7%)*	15 (10.0%)	56 (37.3%)
14. Electrons do not fall into the nucleus as the force attracting the electrons towards the nucleus is balanced by the force repelling the nucleus from the electrons.	87 (58.0%)	13 (8.7%)	50 (33.3%)*
15. The third ionization energy is greater than the second as there are less electrons in the shell to share attraction from the nucleus.	83 (55.3%)	4 (2.7%)	63 (42.0%)*
16. The force pulling the outermost electron towards the nucleus is greater than the force pulling the nucleus towards the outermost electron.	63 (42.0%)	13 (8.7%)	74 (49.3%)*
17. After the atom is ionized, it then requires more energy to remove a second electron because once the first electron is removed the remaining electrons receive an extra share of the attraction from the nucleus.	103 (68.7%)	7 (4.7%)	40 (26.7%)*
18. The atom would be more stable if it 'lost' an electron.	138 (92.0%)	1 (0.7%)	11 (7.3%)*
19. The eleven protons in the nucleus give rise to a certain amount of attractive force that is available to be shared between the electrons.	103 (68.7%)	18 (12.0%)	29 (19.3%)*
20. The atom would become stable if it either lost one electron or gained seven electrons.	120 (80.0%)	3 (2.0%)	27 (18.0%)*

*: correct responses

Table 11

Percentage of Chemistry 1320 Students with Specific Misconceptions Identified From the Instrument EN

	Incorrect %
Alternative notion of stability	
18. The atom would be more stable if it 'lost' an electron.	92.0%
20. The atom would become stable if it either lost one electron or gained seven electrons.	80.0%
12. If the outermost electron is removed from the atom it will not return because there will be a stable electronic configuration.	76.7%
4. Only one electron can be removed from the atom, as it then has a stable electronic configuration.	59.3%
3. The atom will spontaneously lose an electron to become stable.	32.2%
1. Energy is required to remove an electron from the atom.	10.0%
Alternative electrostatic principle – conservation of force	
17. After the atom is ionized, it then requires more energy to remove a second electron because once the first electron is removed the remaining electrons receive an extra share of the attraction from the nucleus.	68.7%
19. The eleven protons in the nucleus give rise to a certain amount of attractive force that is available to be shared between the electrons.	68.7%
15. The third ionization energy is greater than the second as there are less electrons in the shell to share the attraction from the nucleus.	55.3%
Applying Coulombic principle	
14. Electrons do not fall into the nucleus as the force attracting the electrons towards the nucleus is balanced by the force repelling the nucleus from the electrons.	58.0%
6. Each proton in the nucleus attracts one electron.	54.7%
16. The force pulling the outermost electron towards the nucleus is greater than the force pulling the nucleus towards the outermost electron.	42.0%
13. The force on an innermost electron from the nucleus is equal to the force on the nucleus from an innermost electron.	37.3%
8. The nucleus is attracted towards the outermost electron less than it is attracted towards the other electrons.	26.4%
5. The nucleus is not attracted to the electrons.	20.0%

Table 12

Percentage of Chemistry 1320 Students with Specific Explanations for Increase in Ionization Energy Identified From the Instrument EN

	Incorrect %
Explanations for Increase in Ionization Energy	
17. After the atom is ionized, it then requires more energy to remove a second electron because once the first electron is removed the remaining electrons receive an extra share of the attraction from the nucleus (Scientifically incorrect).	68.7%
11. After the atom is ionized, it then requires more energy to remove a second electron because it would be removed from a positive species.	58.7%
7. After the atom is ionized, it then requires more energy to remove a second electron because the second electron experiences less shielding from the nucleus.	50.7%
9. After the atom is ionized, it then requires more energy to remove a second electron because the second electron is in a lower energy level.	46.0%
10. After the atom is ionized, it then requires more energy to remove a second electron because it experiences a greater core charge than the first.	18.7%
2. After the atom is ionized, it then requires more energy to remove a second electron because the second electron is nearer the nucleus.	18.0%

atom" (item 1), and 32.2% of respondents agreed that "the atom will spontaneously lose an electron to become stable" (item 3). This contradiction indicates that many participants only attributed the notion of stability to the idea of configuration or full shells and failed to connect the concept to the concept of energy.

An alternative electrostatic principle – Conservation of force. Items 15, 17, and 19 were designed to reflect the idea of "conservation of electrostatic force", which is a misconception that some students apply on the interaction among a nucleus and electrons (Taber, 2003). Although more energy is required to remove the second electron from a sodium ion as it is closer to the nucleus, experiences a larger core charge, and is being removed from a more positive species, the removal of the second electron does not increase the attraction to the nucleus experienced by the other electrons (Taber, 2002b).

About two-thirds (68.7%) of the participants in this study agreed that "the eleven protons in the nucleus gives rise to a certain amount of attractive force that is available to be shared between the electrons" (item 19), and "after the atom is ionized, it then requires more energy to remove a second electron because once the first electron is removed the remaining electrons receive an extra share of the attraction from the nucleus" (Item 17). In addition, 55.3% of the participants thought that "the third ionization energy is greater than the second as there are less electrons in the shell to share the attraction from the nucleus" (item 15).

Applying the Coulombic principle. Items 5, 6, 8, 13, and 16 were designed to examine whether students apply Coulombic principle when considering interactions among the nucleus and electrons. Twenty percent of the participants thought that "the nucleus is not attracted to the electrons" (item 5). Many students held intuitive ideas thinking "electrons do not fall into the nucleus as the force attracting the electrons towards the nucleus is balanced by the force repelling the nucleus from the electrons" (58%, item 14), or "each proton in the nucleus attracts one electron" (54.7%, item 6). Some students possessed ideas that obey the Coulombic principle thinking, "the force pulling the outermost electron towards the nucleus is greater than the force pulling the nucleus towards the outermost electron" (42%, item 16) or "the nucleus is attracted towards the outermost electron less than it is attracted towards the other electrons" (26.4%, item 8). The failure of applying the Coulombic principle in their explanation of nucleus-electron interaction was also evident by 37.3% of the participants who rejected the idea that "the force on an innermost electron from the nucleus is equal to the force on the nucleus from an innermost electron" (item 13).

Items 17, 11, 7, 9, 10, and 2 were designed to probe students' explanations about the nucleus-electron interaction in terms of an increase of ionization energy. Five of the six items (except item 17) were scientifically correct. Two-thirds (68.7%) of the participants responded that that "after the atom is ionized, it then requires more energy to remove a second electron because once the first electron is removed, the remaining electrons receive an extra share of the attraction from the nucleus" (Item 17) (Table 12). This also indicates an alternative conception about the conservation of electrostatic force (items 17, 19, 15) (Table 11).

Only 58.7% of the participants rejected an idea that "after the atom is ionized, then it requires more energy to remove a second electron because it would be removed from a positive species" (item 11). In addition, 50.7% of the students abandoned ideas that "the second electron experiences less shielding from the nucleus" (item 7), and "the second electron is in a lower energy level" (46.0%, item 9). However, about four-fifths of the students thought that an increase of the second ionization energy was because the second electron "experiences a greater core charge than the first [electron]" (18.7% rejected this idea, item 10) and because it is "nearer the nucleus" (18% rejected this idea, item 2) (Table 12).

Instruments CB and GP

Because conceptions of chemical bonding, molecular geometry, and molecular polarity are closely associated with each other, items of instruments CB and GP were combined for discussions. Table 13 indicated percentages of participants correctly answering items of two-tier questions. Items were rearranged into categories based on conceptions involved. These categories included: (1) octet rule, (2) chemical bond and

Table 13

The Percentage of Chemistry 1320 Students Correctly Answering the First Part and Both Parts of the Instruments CB (7 items, n = 147) and GP (15 items, n = 124)

	Percentage of Chemistry 1320 students correctly answering		
Instrument Items numbered	Content part	Reason part	Both parts
Octet Rule			
GP – 7	87.8	69.9	66.7
Chemical Bond and Valence Electron			
CB – 4	91.8	91.1	89.0
CB – 5	79.6	76.9	74.8
Electronegativity and Bond Polarity			
CB – 1	59.9	64.6	56.5
CB – 2	68.0	46.3	37.4
CB – 7	92.5	73.5	72.1
GP – 10	72.6	48.4	39.5
Molecular Shape			
GP – 1 (NB_3)	45.6	46.4	21.6
GP – 11 (N_2Cl_4, VSEPR theory)	48.4	50.8	33.1
GP – 3 (SCl_2)	71.2	47.2	44.0
GP – 9 (VSEPR theory)	76.6	51.6	46.0
GP – 5 ($COCl_2$)	73.6	20.8	18.4
Polarity of Molecules			
GP – 2	79.2	38.4	26.4
GP – 6 (geometry vs. bond polarity)	75.8	57.3	53.2
Intermolecular Force			
CB – 3	78.2	14.3	5.4
GP – 4 ($H_2O_{(liquid)}$ vs. $H_2S_{(gas)}$)	80.6	16.9	12.9
GP – 8 (OF_2 vs. CF_4)	51.6	36.3	26.6
Lattices			
CB – 6	27.2	30.6	20.4

valence electron, (3) electronegativity and bond polarity, (4) molecular shape, (5) polarity of molecules, (6) intermolecular force, and (7) lattices. When only considering the content part of the items, percentages of students' correct responses ranged from 27.2% to 91.8%. When both content and reason parts were considered, the percentages of correct responses decreased, ranging from 5.4% to 89.0%.

When comparing percentages of correct responses for content part and both parts of the two-tier items by categories, the comparisons reveal a large gap (about 30% of correctness) on items of electronegativity and bond polarity (CB-2, GP-10, & 6), molecular shape (item GP-1, GP-3, GP-9), and a greater gap (greater than 50% of correctness) on molecular polarity (e.g., item GP-2 and GP-4) and intermolecular force (GP-3). The decrease of correct percentages from the content part to both parts of two-tier items suggests that students applied alternative conceptions, but derived a correct content response (Peterson& Treagust, 1989). This gap also indicates that traditional test items written to address merely the content responses were not able to diagnose the level of student understanding.

Combinations of an incorrect content choice and/or incorrect reason choice indicated students' misconceptions about covalent bonding, molecular structure, and polarity. For example, when a participant chose incorrect answers (2) for the content part and (B) for the reason part on item CB-5, the choice combination is indicated as CB-5 [2B]). Misconceptions were identified if they existed in at least 10% of the student samples. Nineteen misconceptions identified from instruments CB and GP were grouped into categories as chemical bonds, molecular shape, polarity of molecules, intermolecular forces, and lattices (Table 14).

The octet rule and chemical bonds. Regarding students' understanding about the octet rule (item GP-7), 87.8% of the students responded that "the octet rule is used to

Table 14

Percentage of Chemistry 1320 Students with Specific Misconceptions Identified from the Instruments CB (n = 147) and GP (n = 124)

Misconceptions	Choice Combination	%
Chemical bonds		
1. Electron sharing occurs when forming an ionic bond.	CB-5 [2B]	16.3%
2. When an atom with high electronegativity forms a bond, a double or triple bond is always present; therefore, the structure of the N_2Cl_4 molecule is $Cl_2N{=}NCl_2$.	GP-11 [2A]	12.9%
Bond polarity		
1. Equal sharing of the electron pair occurs in all covalent bonds.		
• As hydrogen and fluorine form a covalent bond the electron pair must be shared equally.	CB-1 [2B]	27.2%
• The kind of bonding to make the water molecule (H_2O) is polar covalent bonding, because hydrogen and oxygen share electrons equally.	CB-7 [2C]	10.9%
2. Sulfur is partially positive in the S-Cl bond of SCl_2 because the sulfur atom donates an electron to the chlorine atom resulting in the formation of S^+ and Cl^- ions.	GP-10 [1A]	16.9%
3. The polarity of a bond is dependent on the number of valence electrons in each atom involved in the bond.		
• A polar covalent bond forms because oxygen has six outer shell electrons and fluorine has seven outer shell electrons; therefore fluorine is partially negative and oxygen is partially positive.	CB-2 [2B]	19.0%
4. Relate partial charges in a polar bond due to different electronegativity of atoms to formation of ions.		
• The sulfur atom is partially negative (δ^-) as it can form as S^{2-} ion, whereas chlorine can only form a Cl^- ion in a SCl_2 molecule.	GP-10 [2B]	12.1%
• Oxygen is partially negative in an oxygen-fluorine bond because the oxygen atom forms an O^{2-} ion, whereas fluorine forms as F^- ion.	CB-2 [1D]	10.9%
Molecular shape		
1. Bond polarity determines the shape of a molecule.		
• The shape of the $COCl_2$ is due to the stronger polarity of the C=O double bond in the molecule.	GP-5 [2C]	24.0%
• The shape of nitrogen bromide is <u>trigonal planar</u>, because nitrogen forms three bonds which equally repel each other to	GP-1 [1A]	18.4%

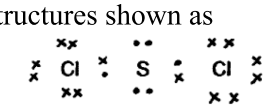
form a trigonal planar shape.

- The shape of nitrogen bromide is <u>trigonal pyramidal</u>, because the polarity of each nitrogen-bromine bond determines the shape of the molecule. — GP-1 [2C] — 10.4%

2. Electronegativity of each atom determines the shape of a molecule. — GP-5 [2A] — 16.0%
3. Repulsion between non-bonding pairs determines the shape of a molecule. — GP-3 [1B] — 19.2%
4. Repulsion between the atoms in the molecule determines the shape of a molecule. — GP-9 [2D] — 13.7%
5. Include non-bonding electron pairs when describing molecular shape; therefore the shape of nitrogen bromide is tetrahedral. — GP-1 [3B] — 21.6%

Polarity of Molecules

1. Non-polar molecules form when the atoms in the molecule have similar electronegativities; polar molecules form when the atoms in the molecule have great difference of electronegativity.
    - Chlorine trifluoride (ClF_3) is a non-polar molecule because there is very little difference between the electronegativities of Cl and F. — GP-6 [2D] — 16.1%
    - The similar electronegativities of oxygen and fluorine result in OF_2 being non-polar. — CB-8 [1B] — 12.1%
    - The large electronegativity difference between carbon and fluorine atoms results in CF_4 being polar. — CB-8 [2C] — 10.5%
2. Polar molecules form when there are non-bonding electrons in the molecule.
    - OF_2 is a polar molecule, because non-bonding electrons on an atom in the molecule produce a dipole and hence a polar molecule. — GP-2 [2C] — 37.6%
    - The electron pair repulsion theory is used to determine the shape of a molecule. Non-bonding electrons determine the polarity of a molecule. — GP-9 [2A] — 12.9%
3. Polar molecules form when high electronegative atoms present. — GP-6 [1B] — 16.1%
4. Determine molecular shape and polarity merely based on representations (e.g. chemical formula or Lewis dot structure).
    - The molecule SCl_2 is linear. The two sulfur-chlorine bonds are equally repelled to linear positions because SCl_2 has an electron dot structures shown as — GP-3 [2C] — 17.6%



    - The shape of molecule Cl–:S: –Cl is linear. — GP-13 [C] — 19.4%
    - The shape of molecule Cl–Sn: –Cl is linear. — GP-13 [B] — 12.9%
    - The shape of molecule SCl_4 is tetrahedral. — GP-12 [B] — 15.3%
    - The shape of molecule $SeCl_4$ is tetrahedral. — GP-12 [C] — 11.3%

• H_2S is non-polar.	GP-14 [B]	25.0%
• CCl_2F_2 is non-polar.	GP-14 [C]	23.4%
• O=O:–O is non-polar.	GP-15 [A]	18.5%
Intermolecular Force		
1. Silicon carbide has strong intermolecular forces, because a large amount of energy is required to break the intermolecular forces in the silicon carbide lattice.	CB-3 [2B]	65.3%
2. The difference in strength of the intermolecular forces (comparing $H_2O_{(liquid)}$ and $H_2S_{(gas)}$) is due to the difference in strength of O-H and S-H covalent bond.	GP-4 [2A]	29.8%
3. The strength of intermolecular forces of a compound is greater when there are more polar bonds present in each molecule.	CB-8 [2A]	10.5%
• If OF_2 and CF_4 are compared, strength of the intermolecular forces is greater between CF_4 molecules, because there are four polar bonds in CF_4 and only two in OF_2.		
4. Covalent bonds are broken when a substance changes shape. The harder covalent bonds to be broken, the greater the intermolecular forces.	GP-4 [2B]	29.8%
Ionic Lattices		
1. After sodium atom donates its valence electron to the chloride atom, the sodium ion forms a molecule with the chloride ion.	CB-6 [1B]	33.3%
2. The sodium atom shares a pair of electrons with the chlorine atom to forms a simple molecule.	CB-6 [1A]	21.8%

determine the number of bonds an atom forms," and 66.7% of students were correct on both parts. Results of items CB-4 and CB-5 showed that students had a good understanding about the role of valence electrons in forming chemical bonds (89.0% for both parts, item CB-4) and ionic bonds (74.8% for both parts, item CB-5) (Table 13). However, analyses of misconceptions indicated that there were still 16.3% of the participants who related electron-sharing to the formation of ionic bonds (combination CB-5 [2B], Table 14).

Bond polarity. Items CB-1, 2, 7, and GP-10 were designed to diagnose students' understanding about the relationship between electronegativity and bond polarity (Table 13). Most of the students who indicated that the shared electron pair in the HF molecule should be closer to the fluorine atom (59.9% for content part, item CB-1) gave the correct reason as "fluorine has a stronger attraction" (56.5% for both part, item CB-1). Items CB-2, 7, and GP-10 required students to associate an concept of bond polarity to electronegativity; and students' responses to these three questions indicated that about 20.4% (item CB-7), 30.6% (item CB-2), to 33.1% (item GP-10) of the students held alternative conceptions attributing bond polarity to other reasons.

Analysis of the alternative responses revealed three misconceptions in Table 14 under the heading of bond polarity. The first misconception indicated that students correctly related electron sharing to formation of covalent bonds, but thought that the electron pair was shared equally in all covalent bonds without considering the influence of electronegativity (combination CB-1 [2B], 27.2%; CB-7 [2C], 10.9%). For 16.9% of students (combination GP-10 [1A]) who considered the difference of electronegativity of atoms in the S-Cl bond of SCl_2, in their reasoning, they misinterpreted the unequal share of electrons as the sulfur atom donates an electron to the chlorine atom resulting in the formation of S^+ and Cl^- ions. Nineteen percent of the students (combination CB-2 [2B]) determined bond polarity was based on the number of valence electrons in each atom involved in the bond. Therefore, fluorine should be assigned as partially negative in an oxygen-fluorine covalent bond because it has seven valence electrons in its outer shell compared with oxygen that has only six valence electrons. Combination GP-10 [2B] indicated that 12.1% of the students considered the sulfur atom is partially negative (δ^-) in a SCl_2 molecule because it can form S^{2-} ion as a greater magnitude of negative charges compared with chlorine that can only form a Cl^- ion. Similar results can be found when students determined the partial charges of an oxygen–fluorine bond (combination CB-2 [1D], 10.9%).

Molecular shape. Regarding the concept of molecular shape, both items GP-3 and GP-9 focused upon the concept of electron repulsion theory (Table 14). The percentages of students' correct responses to the content and both parts for these two questions reflected a similar pattern. Item GP-1 and GP-11 addressed similar concepts of electron repulsion theory except that they used molecules that students were not familiar with from Chemistry 1320. Due to the use of unfamiliar molecules, there was a 13%~25% decline on students' correct responses for the content part and both parts of items GP-1 and GP-11, compared with items GP-3 and GP-9 using simple molecules. Item GP-5 examined an application of electron repulsion theory on a molecule containing a double bond. Although 73.6% of the students correctly predicted the shape of $COCl_2$, only 18.4% of students chose an appropriate reason to support their prediction.

Five misconceptions were identified regarding molecular shape (Table 14). Students considered only one of the following factors when determining the shape of a molecule: bond polarity (combinations GP-5 [2C], 24.0%; GP-1 [1A], 18.4%; and GP-1 [2C], 10.4%), electronegativity of each atom, (combination GP-5 [2A], 16.0%), repulsion between non-bonding pairs (combination GP-3 [1B], 19.2%), or repulsion between the atoms in the molecule (combination GP-9 [2D], 13.7%). About 20% of the students included non-bonding electron pairs when describing the molecular shape and determined the shape of nitrogen bromide as tetrahedral structure.

Polarity of molecules. Items GP-2 and GP-6 diagnosed factors that students considered to determine whether a molecule is polar or non-polar (Table 13). More than

75% of the students identified polar molecules successfully, yet only 26.4% of the students applied the correct reasoning (Item GP-2).

Analyses of misconceptions revealed that students neglected the symmetrization of molecular geometry when determining polarity of molecules and attributed polarity of molecules to either (1) presence of atoms with high electronegativity (combination GP-6 [1B], 16.1%), (2) large difference of electronegativity between atoms (combinations GP-6 [2D], 16.1%; CB-8 [1B], 12.1%; CB-8 [2C], 10.5%), or (3) the presence of non-bonded electron pairs (combinations GP-2 [2C], 37.6%; GP-9 [2A], 12.9%) (Table 14). In addition, 11.3% to 25% of the students determined molecular shapes and polarity merely based on 2D representations (e.g., chemical formula or Lewis dot structure).

Intermolecular forces. Question CB-3 was designed to assess students' understanding about covalent networks. About 78% of the students correctly related the high melting and boiling points of silicon carbide to its strong intermolecular forces (item CB-3) (Table 13). However, 65.3% of the students associated the properties as high melting and boiling points that required a large amount of energy to break the intermolecular force (combination CB-3 [2B], Table 14), and only 5.4% of the students associated these properties to its characteristic of the covalent network. Items GP-4 and GP-8 were designed to diagnose students' reasoning to determine the strength of intermolecular force (Table 13). Item GP-4 showed that giving a cue to indicate states of the compound (e.g., $H_2O_{(liquid)}$ and $H_2S_{(gas)}$) in the question increased the percentage of correct responses on the content part (80.6%) compared to item GP-8 merely giving chemical formulas as OF_2 and CF_4 (51.6%). However, when students' responses to both parts were examined, only 12.9% and 26.6% of the students attributed molecular polarity to a correct reason.

About 30% of participants in this class possessed a misconception of considering only the strength of covalent bonds when determining the strength of intermolecular forces (combination GP-4 [2A], Table 14). About 10% of the students associated the number of polar bonds in a molecule with the strength of intermolecular forces thinking CF_4 has a greater intermolecular force than OF_2 because there are four polar bonds in CF_4 and only two in OF_2 (combination CB-8 [2A]). The other major misconception was students thought covalent bonds were broken when a substance changed shape (combination GP-4 [2B], 29.8%). Students who possessed this misconception thought that the H_2S compound had weaker intermolecular forces than H_2O compound because the bonds in H_2S were easier to break.

Ionic lattices. Surprisingly, 72.8% of the students considered sodium chloride (NaCl) existing as a molecule (item CB-6). Only 20.4% of the students associated sodium chloride to a lattice structure consisting of sodium and chloride ions (Table 13). Analyses of misconceptions showed that 33.3% of students held a conflicting idea thinking that the sodium ion forms a molecule with the chloride ion by donating its valence electron (combination CB-6 [1B], Table 14). In addition, 21.8% of the students considered that the sodium atom shares a pair of electrons with the chlorine atom to form a simple molecule (combination CB-6 [1A]).

Inferential Statistics

This section describes the tests of the null hypotheses using one-way ANOVA. Independent variables of this study included gender (male and female), number of chemistry courses participants enrolled prior to Chemistry 1320 (n = 0, 1, 2, and ≥ 3), scores of four course exams, and final course grade. Dependent variables are students' scores on instrument EN, instrument CB, and instrument GP.

The first null hypothesis tested for differences between male and female general chemistry students on their course performances in terms of exams 1, 2, 3, final exam, and course grade. The one-way ANOVA demonstrated no significant differences for the main effect of gender (Exam 1, $F(1, 141) = 0.49$, $p > 0.05$; Exam 2, $F(1, 140) = .18$, $p > .05$; Exam 3, $F(1, 140) = 2.50$, $p > .05$; Final exam, $F(1, 140) = 1.31$, $p > .05$; Course grade, $F(1, 140) = 0.28$, $p > .05$) (Table 15). This indicates that there was no significant difference between male and female students on their mean scores of their exams 1, 2, 3, final examine, and course grade. Therefore, the first null hypothesis was not rejected.

The second null hypothesis tested for differences between male and female students on their score of instrument EN. The one-way ANOVA demonstrated a significant difference for the main effect of gender, $F(1, 133) = 8.56$, $p < .05$ (Table 16). However, the effect size (partial Eta squared = .06) was small. This indicates that there was a significant difference between male and female students on their mean scores of instrument EN. Therefore, the second null hypothesis was rejected.

The third and fourth null hypotheses were developed to test for differences between male and female students on their scores of instruments CB and GP, respectively. The one-way ANOVA demonstrated no significant differences for the main effect of gender for instruments CB, $F(1, 129) = 0.08$, $p > .05$, and GP, $F(1, 109) = 0.41$, $p > .05$ (Table 16). This indicates that there was no significant difference between male and female Correlations between scores of instruments EN, CB, GP, exams 1, 2, 3, final exam, and

Table 15

One-way ANOVA between Gender for Scores on Exams 1, 2, 3, Final Exam, and Course Grade

		SS	*df*	*MS*	*F*	*p*
Exam 1	Between Groups	9.49	1	9.49	.049	.83
	Within Groups	27201.35	141	192.92		
	Total	27210.84	142			
Exam 2	Between Groups	36.66	1	36.66	.183	.67
	Within Groups	28049.26	140	200.35		
	Total	28085.92	141			
Exam 3	Between Groups	590.29	1	590.29	2.504	.12
	Within Groups	33004.95	140	235.75		
	Total	33595.25	141			
Final Exam	Between Groups	200.41	1	200.41	1.307	.26
	Within Groups	21468.76	140	153.35		
	Total	21669.16	141			
Course Grade	Between Groups	24.83	1	24.83	.284	.60
	Within Groups	12229.42	140	87.35		
	Total	12254.25	141			

Table 16

One-way ANOVA between Gender for Scores on Instruments EN, CB, and GP

		SS	*df*	*MS*	*F*	*p*
Instrument EN	Between Groups	67.21	1	67.21	8.56	.004
	Within Groups	1044.52	133	7.85		
	Total	1111.73	134			
Instrument CB	Between Groups	.18	1	.18	.08	.78
	Within Groups	297.73	129	2.31		
	Total	297.91	130			
Instrument GP	Between Groups	4.58	1	4.58	.41	.53
	Within Groups	1231.15	109	11.30		
	Total	1235.73	110			

students on their mean scores of instrument CB and of GP, respectively. Therefore, the third and the fourth null hypotheses were not rejected.

course grade were also computed. The correlation coefficients indicated that scores on instrument EN only had a weak correlation with scores on instruments CB, GP, as well as exams 1, 2, 3, final exam, and course grade. Scores on instruments CB and GP each had moderate correlation with four course exams, and course grade. Scores on exams 1, 2, 3, final exam, and course grade were highly correlated (Table 17).

Table 17

Correlations between Scores of Instruments EN, CB, and GP, Exams 1, 2, 3, Final Exam, and Course Grade (n=142)

Subscale	1	2	3	4	5	6	7	8
1. Instrument EN	—	.33*	.18	.24*	.30*	.34*	.27*	.34*
2. Instrument CB		—	.50*	.45*	.44*	.40*	.40*	.44*
3. Instrument GP			—	.39*	.41*	.35*	.35*	.40*
4. Exam 1				—	.51*	.56*	.59*	.68*
5. Exam 2					—	.56*	.67*	.76*
6. Exam 3						—	.63*	.74*
7. Final Exam							—	.91*
8. Course Grade								—

*: Correlation is significant at the .01 level (2-tailed).

The fifth null hypothesis was developed to test for correlations between participants' exams and final score for Chemistry 1320 and their scores of the instruments EN, CB, and GP. The correlation coefficients indicated that the scores on instrument EN only had a weak significant correlation with scores of instruments CB, GP, as well as exams 1, 2, 3, final exam, and course grade. Scores on instruments CB and GP both have moderate significant correlation with four course exams, and course grade. Scores on exams 1, 2, 3, final exam, and course grade were highly correlated with each other. Therefore, the fifth null hypothesis was rejected (Table 17).

The sixth null hypothesis was developed to test for difference between participants who had enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their course performances in terms of exams 1, 2, 3, final exam, and course grade. The one-way ANOVA showed no statistically significant difference for the main effect of the number of previous chemistry courses (Exam 1, $F\ (2, 124) = .20$, $p > .05$; Exam 2, $F\ (2, 123) = .59$, $p > .05$; Exam 3, $F\ (2, 123) = .55$, $p > 0.5$; Final exam, $F\ (2, 123) = .17$, $p > .05$; Course grade, $F\ (2, 123) = .18$, $p > .05$) (Table 18). This indicates that there was no significant difference between participants who previously enrolled in 0, 1, 2, and ≥ 3 chemistry courses on their performance on exams 1, 2, 3, final examine, and course grade. Therefore, the sixth null hypothesis was not rejected.

The seventh, eighth, and ninth null hypotheses were developed to test for differences between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their scores of instruments EN, CB, and GP, respectively. The one-way ANOVA showed no significant difference for the main effect of the number of previous chemistry courses for instrument EN, $F\ (2, 119) = .08$, $p > .05$, instrument CB, $F\ (2, 116) = .35$, $p > .05$, and GP, $F\ (2, 100) = .59$, $p > .05$ (Table 19). This indicates that there was no significant difference between participants who enrolled in 0, 1, 2, and ≥ 3 previous chemistry courses on their mean scores of instruments EN, CB, and GP, respectively. Therefore, the seventh, eighth, and ninth null hypotheses were not rejected.

Table 18

One-way ANOVA between the Number of Previous Chemistry Course for Scores on Exams 1, 2, 3, Final Exam, and Course Grade

		SS	*df*	*MS*	*F*	*p*
Exam 1	Between Groups	76.44	2	38.22	.20	.82
	Within Groups	23445.61	124	189.08		
	Total	23522.05	126			
Exam 2	Between Groups	211.67	2	105.83	.59	.56
	Within Groups	21987.54	123	178.76		
	Total	22199.21	125			
Exam 3	Between Groups	248.36	2	124.18	.55	.58
	Within Groups	27950.26	123	227.24		
	Total	28198,61	125			
Final Exam	Between Groups	56.87	2	28.44	.17	.84
	Within Groups	20267.93	123	164.78		
	Total	20324.80	125			
Course Grade	Between Groups	31.73	2	15.86	.18	.84
	Within Groups	11153.13	123	90.68		
	Total	11184.86	125			

Table 19

One-way ANOVA between the Number of Previous Chemistry Course for Scores on Instruments EN, CB, and GP

		SS	*df*	*MS*	*F*	*p*
Instrument NE	Between Groups	1.47	2	.73	.08	.91
	Within Groups	1036.40	119	8.71		
	Total	1037.87	121			
Instrument CB	Between Groups	1.53	2	.77	.35	.71
	Within Groups	256.69	116	2.21		
	Total	258.22	118			
Instrument GP	Between Groups	12.44	2	6.22	.59	.56
	Within Groups	1053.42	100	10.53		
	Total	1065.86	102			

Qualitative Phase

Findings of General Chemistry Students' Mental-Modeling Ability, Conceptual Frameworks, and Mental Models about Molecular Geometry and Polarity

Based on qualitative findings of the study, level of content knowledge and mental-modeling ability were two factors that emerged from analyses of students' mental models about molecular geometry and polarity. Both factors influenced the processes of construction and use of mental models, and features of students' mental models are considered as outcomes resulting from the interaction between an individual's content knowledge and mental-modeling ability. Within and cross-case analyses including eight student interviews were conducted using grounded theory. Guided by research questions, these eight cases were analyzed to characterize students' mental-modeling ability, to portray the quality and content of conceptual frameworks, and to illustrate features of mental models that students generated when thinking about problems of molecular geometry and polarity.

Based on the quality and content of the students' conceptual frameworks about molecular shape, polarity, and the prerequisite concepts, the eight interview participants were categorized into three levels: high, moderate, and low content knowledge groups. Similarly, these participants' were divided into three levels of mental-modeling ability according to their ability to construct and use their mental models. Table 20 shows the categorization for levels of content knowledge and mental-modeling ability for the eight interview participants based on their interview analyses.

To organize this section, I start with discussions on characteristics of students' mental-modeling ability in the high, moderate, and low groups. These four

Table 20

Categorization for Levels of Content Knowledge and Mental-Modeling Ability for Eight Participants

	High content knowledge	Moderate content knowledge	Low content knowledge
High mental-modeling ability (HMMA)	JS, RE		
Moderate mental-modeling ability (MMMA)	CR	AM, SD	
Low/No mental-modeling ability (LMMA)			TA, KA, JT

characteristics emerged from the cross-case analysis that portrayed a sophisticated mental-modeling process when solving molecular polarity problems. These four characteristics were then assembled to form a protocol (Table 21) that was used to recode and score the eight participants' mental-modeling ability. Based on their scores, these eight students were assigned into high mental-modeling ability (HMMA), moderate mental-modeling ability (MMMA), and low mental-modeling ability (LMMA) groups. For each level of mental modeling ability, I provide excerpts from the interviews to demonstrate how the four characteristics in the protocol illustrate an individual's mental-modeling ability and how possessing a different level of mental-modeling ability influences his or her thinking processes while solving problems related to molecular geometry and polarity.

Next, I describe characteristics of students' conceptual frameworks in the high, moderate, and low content knowledge groups. Results of analyses for each student's understanding about concepts of molecular geometry, polarity, and prerequisite concepts were organized into three conceptual frameworks: (1) atomic model, (2) chemical bonding, and (3) molecular geometry and polarity. Each student's three conceptual

Table 21

Protocol of Mental-Modeling Ability and Scores of the Mental Modeling Ability for Eight Participants

	Mental-modeling ability							
	High (HMMA)		Moderate (MMMA)			Low (LMMA)		
Characteristics of mental-modeling ability (score)	JS	RE	CR	AM	SD	TA	KA	JT
1a. Generate a mental model w/ and w/o a 2D representation (2 points) 1b. Generate a mental model based on a 2D representation (1 points)	2	2	2	1	1	1	1	0
2a. Manipulate the mental model based on propositions (4 points) 2b. Possess a rigid mental model and conclude that the shape of mental model would not change when a new proposition is added to the model; sometimes need to rely on a concrete model (2 points)	4	4	3	3	2	1	0	0
3. Metacognitively monitor processes of mental modeling (2 points)	2	2	1	0	1	0	0	0
4. Self-check using an alternative approach to test or inspect the mental model to identify errors from the mental model (2 points)	2	2	0	0	0	0	0	0
Total (10 points)	10	10	6	4	4	2	1	0

frameworks were also illustrated by three corresponding concept webs. Examples from students' excerpts and drawings were used to portray their understanding at each level and differences among characteristics of students' conceptual frameworks.

Accuracy and level of details for a mental model reflect outcomes of interactions between content knowledge and mental-modeling ability in a student's mind. Thus, in the last section I explained the criteria in a protocol that was used to evaluate features of students' mental models about H_2S and BF_3. Scores for each participant's mental models are reported to exemplify the outcomes of the interactions between his or her content knowledge and mental-modeling ability.

Characteristics of Students' Mental-Modeling Ability While Thinking About Concepts of Molecular Geometry and Polarity

Four characteristics of mental-modeling ability emerged from the interview analyses that distinguish students in the high, moderate, and low mental-modeling ability groups. The first characteristic describes whether a student generates a 3D mental model when a chemical formula is given without drawing a Lewis structure. Depending on their familiarity with a given molecule, sometimes students were able to determine the Lewis structure of the molecule mentally while generating a 3D mental model; yet other times they relied on creating a 2D Lewis dot structure on paper to provide cues for visualizing a 3D mental model. This characteristic is divided into two levels depending on whether construction of a 2D representation on the paper is needed for mental model construction. Some students used the constructed 2D Lewis structure to provide cues about numbers of lone pairs and bonding pairs that the molecule contained. Some students used the 2D Lewis structure to provide visual cues for molecular geometry and visualized a 3D mental model having the same shape as the 2D Lewis structure. Examples of students' use of 2D Lewis structure are discussed later for HMMA, MMMA, and LMMA groups.

Students in the HMMA group possessed the third and the fourth characteristics which underpinned the individual's metacognitive ability. The third characteristic describes the presence of students' use of metacognition to monitor his or her mental modeling processes. Students' actions of metacognition are outside of the scope of this study. However, approaches such as self-dialogue while solving a problem and evaluating the context of a problem and the necessary information for problem-solving were observed in the students in the HMMA group. The fourth characteristic describes the behavior of an individual's self-checking using an alternative approach, such as drawing a Lewis structure on the paper, to verify his or her mental model or answers.

Although the levels of mental modeling abilities are described as categories (high, moderate, and low), they can be thought of as a continuum with the LMMA group reflecting students who do not have or have very limited ability to generate and use mental models while the HMMA students reflect the most sophisticated ability (observed among the interview participants). HMMA students not only construct and use mental models, but also evaluate their mental models and monitor the mental-modeling processes. In the following subsections, I describe mental-modeling ability for high, moderate, and low groups referring to the four characteristics in the Table 21.

High Mental-Modeling Ability Group (HMMA Group)

Students in the HMMA group could construct a mental model of a given molecule with or without a 2D representation (Characteristic 1a). HMMA students were able to generate a 3D mental model of a given chemical formula (e.g. BF_3) without drawing a 2D

Lewis dot structure on a paper. While the students talked-aloud during problem-solving processes, they gestured with their hands in the air to label each imaginary atom as boron and fluorine atoms, as well as correctly indicated relative positions of the atoms spatially. After the imaginary molecule was constructed, the students were able to change their reference point to imagine what the molecule would look like from different angles. Ferk et al. (2003) describes this visualization skill as spatial orientation. They could also rotate the model to examine the spatial structure of the molecule from different angles if necessary, in Ferk et al.'s term, spatial relations. RE's descriptions about visualization of a BF_3 molecule demonstrates this characteristic:

> What's in my head? Okay, um…basically what I did was I kind of make a Lewis structure in my head. Like I said, okay,…you have a boron and three fluorines. So…the boron's the one that's going to be in the middle. Then I had three fluorines and I pictured, okay, if I had three more atoms what kind of shape is that going to make? And I just kind of pictured like four dots with one in the middle making a shape and I said, okay, that's going to put one here, one here, and one here. So I'm going to have a triangular shape. [25:49-26:10] (RE, interview)

RE further described how she could perform visualization skills on a mental model:

> …when I think of molecules in my head, the only way that they turn is, like, kind of if you were on a computer and you were looking at a 3D image and you just like spin it to look at it from the different angles…Like, just so I can see the different angles and how the shape is and stuff like that. [4:12-4:32] (RE, interview)

Students in the HMMA group were able to reconstruct, manipulate, or adjust a mental model accordingly by imposing propositions or conditions of the problem on the model (Characteristic 2a). These students were able to reconstruct, manipulate, or adjust parts of the mental model, accordingly, by applying propositional statements to the model. Students may perform this action consciously or subconsciously while constructing or adjusting their mental model. Either way, they were able to explain and justify their actions, retrospectively, with the propositional statements that were imposed on the model. I use RE's case to illustrate this characteristic of mental-modeling ability:

> I: If I have a boron trifluoride, is it a polar or non-polar molecule?
>
> RE: If I just think about it off the top of my head, like I can picture the boron's going to be in the middle. There's three fluorides. And they are going to make…a triangular shape, they're all going to be coming out from the bottom. No it is going to be triangular planar. [23:21-24:10]
>
> RE: And it is going to be in one plane most likely because if there's no lone pairs it is all going to be in the same plane. And then I said, okay, then if I had these three and they're going to be evenly spaced apart…you know the angles are all going to be the same then the pulls [dipole moments] are going to be towards the fluorines. And it is going to pull, like one's pulling this way, one's pulling this way, one's pulling this way. And it is going to cancel, they're all going to cancel out. [26:10-27:00] (RE, interview)

RE started off visualizing the BF_3 molecule with three B–F bonds coming from the bottom of the boron atom. She soon realized that there were no lone pairs or bonds on top of the boron atom. Therefore, RE adjusted her mental model from a trigonal pyramidal shape to a trigonal planar shape by imposing the VSEPR model to her model, thinking the three B–F bonds would repel each other and stay as far apart from each other as possible. In the next step, RE applied the concept about bond dipole, resulting from the electronegativity difference between boron and fluorine atoms, to each B–F bond with notions of the direction and magnitude of the bond polarity. Applying appropriate and correct propositions to a functional mental model, RE was able to correctly infer molecular polarity by summing the overall dipole moments.

These HMMA students' mental models were functional. These students incorporated conditions of a problem or phenomenon and the propositional statements they considered appropriate to the mental model construction. Therefore, the mental models served a function to illustrate considerations that these students imposed on the mental model. Once the mental model was constructed, the mental model was flexible which allowed students to apply an additional condition or proposition to the model and to adjust it accordingly. The functional mental model increases the chances for students to derive a model that represents more accurate spatial information, if the propositions that students possess are accurate in the first place. With the functional mental model, both students in the HMMA group were able to use a model that contained accurate spatial information as a base for an inference. In the following conversations, JS's case provided strong evidence of how he applied appropriate propositions to a constructed mental model at two different times and derived an answer that was beyond his existing knowledge:

> I: What would be the bond angle [of H_2S]?
> JS: The bond angle? …between the 2 sulfurs it'd be less than 109.5. Just a little less than 109.5.
> I: Why is it less?
> JS: Because if all of these were equally apart then it would be 109.5. But we know that these electron pairs [lone pairs] push out more, so they squeeze these [H-S bonds] a little bit closer so it is a little bit less than 109.5. [2:43-3:12]
> I: If we replace the 2 hydrogen atoms of H_2S with two chlorines, would the bond angle change?
> JS: I do not think the bonding would – it does make sense that it would change. I do not think I've ever been taught that it would, but it makes sense that it would because there would be more electrons on a chlorine atom than there are on a hydrogen, and you would kind of think that those electrons would want to repel each other. [13:25-14:04] (JS, interview)

HMMA students were able to recognize their approaches to the problem and constantly monitor their processes of reasoning and construction of mental models (Characteristic 3). Throughout the entire processes of mental model construction and problem-solving, these HMMA students metacognitively monitored their processes of reasoning. The two students in this group each employed different approaches. For example, when determining the polarity of BF_3, RE had a series of self-dialogues, posing questions to herself and then answering them during each step of problem-solving process. Also, when RE and JS were asked to build a model of 1, 2-dichloroethane ($C_2H_4Cl_2$), a molecule with novel geometry to the students, they both could recognize and describe their strategy of visualizing the 3D molecular geometry. For instance, RE responded:

> I just kind of say, okay, you know this is got four it is gonna be a tetrahedral…what I did was basically…I divided it in half like…I said, okay, if I just look at this half and then how's that shape gonna be, instead of trying to picture the whole thing at once. I broke it up so that I could see okay, this is how this side is gonna be. And this side is just pretty much the same thing attached to it, so. [2:24] (RE, interview)

I use JS's descriptions about his mental model of BF_3 as another example. During the mental-modeling processes, JS examined the problem: to determine whether BF_3 is a polar or nonpolar molecule. He then constructed and used a mental model that contained only essential features in order to solve the problem.

> JS: This is what I picture. I picture a boron right here and then fluorine, fluorine, fluorine and that's about it. Of course I know that they're bonded. But that's all I really need to know that it is a trigonal planar, because in my picture, if I were drawing electron pairs, I mean if there were some I would add that in my picture. But it is not in my picture because I know that the unshared electron pairs do not exist, so that's all I need to know that they're a trigonal planar. That there are 3 forces, they're equal forces so they equally repel. [22:25-23:10]
>
> I: When this image emerged in your mind can you do something with it? Did you do something with it to help you think about the geometry of BF_3?
>
> JS: In my mind, as far as the geometry it was pretty simple just what I went through before. I knew that there were only three things outside and they were all the same, so I knew they were trigonal planar. And I did not even really…in my mind I did not care whether or not they were moving. It did not really make any difference to me. [24:36-25:09]

Also, these HMMA students self-checked and verified their mental models and answers using an alternative approach if the given molecule was relatively novel to them (Characteristic 4). With the actions of the metacognitive monitoring described as the previous characteristic, HMMA students generally had affirmed the correctness of their mental model and the derived answers at the end of the mental-modeling processes. When the students encountered a molecule which was relatively novel to them, after they derived a conclusion using their mental model, they used an alternative approach, for example, drawing out a Lewis dot structure of the molecule step-by-step and counting numbers of lone pairs and bonding pairs to verify the same process they had done earlier in their mind. Also, they used the 2D Lewis dot structure to inspect and verify their mental model. It was not clear, however, whether or not these students applied propositional statements to the 2D Lewis dot structure for inference before the 2D Lewis structure was used to verify their mental model. The following excerpts described RE's self-checking processes after she had used her mental model to determine that BF_3 is a nonpolar molecule, and she said:

> Now, I could be wrong just thinking that off the top of my head because the things like that, that's the kind of thing that you may end up drawing. Let's see, borons got three…plus 21. [She adds up the overall number of valence electrons.] You may end up drawing it and find that there's a lone pair and that's going to change it a little bit.
>
> (Silence from 24:34 to 24:53) [She is drawing a Lewis structure of BF_3 on the paper]
>
> Okay, so it does not have any lone pairs so…it is gonna be the same thing as what I said. [24:10-25:03] (RE, interview)

She further specified the situation when she would perform this self-checking:

> But if there was one that had lone pairs, I mean except for some of the ones that you see all the time like water, like that one [H_2S] I know exactly what

> the Lewis structure looks like in my head. But stuff that maybe you do not see everyday, I'd have to, like, I might do this in my head, but I'd probably second guess myself. So I'd have to sit down and draw it out just to make sure I was right, and I did not leave something out and get the wrong answer. [25:49-28:10] (RE, interview)

Moderate Mental-Modeling Ability Group (MMMA Group)

Students in the MMMA group constructed a 2D Lewis structure before a mental model was generated. When the students were familiar with the geometry of a given molecule, they could form a mental model without seeing the 2D representation (Characteristic 1b). Before generating a 3D mental model, most students in the MMMA group needed to draw a 2D Lewis dot structure of a given chemical formula in order to count numbers of lone pairs and bonding pairs in the molecule. Once the imaginary molecule was constructed, the students could perform similar visualization operations as their peers in HMMA group to rotate and to examine the imaginary molecule from different angle.

Evidence showed that some students in this group experienced difficulties with perceiving the spatial structure of some molecular geometry in three dimensions. These students were able to visualize a 3D mental image of a molecule as if the molecule had a geometry that they saw frequently in the textbook or in class, for example, a bent molecule that had the same shape as a water molecule. Visualizing a 3D mental model became more difficult for these MMMA students if the molecule had a 3D geometry that was relatively novel to the individual. Visualizing a trigonal planar geometry was particularly difficult for SD. She said:

> They talk about this planar one all the time, which I do not have a good concept of the planar ones. Those are kinda hard cause it almost seems like they're flat but I'm not sure cause we did not do a whole lot of examples where they're like that. [25:26-25:59] (SD, interview)

SD understood the VSEPR model and was able to apply it to some other geometry, but did not comprehend the geometric structure of a trigonal planar. Therefore, SD had difficulty visualizing a 3D mental model by applying the VSEPR model to adjust her mental model and to infer a possible geometry. For SD, whether a specific molecular geometry, for example, a trigonal planar, was available to recall and use in her conceptual framework was critical for visualizing a 3D mental model.

Students in the MMMA group had some degree of ability to manipulate their mental model when compared to students in the HMMA group, but sometimes, these students neglected to review the problem and problem-solving processes carefully. Therefore, they held on to a rigid mental model rather than modifying or adjusting it based on the new condition in the problem (Characteristic 2a & 2b). Mental models of the MMMA students had limited function while they could impose conditions of a problem and propositional statements they considered appropriate to the mental model during the model construction. Once the mental model was constructed, students often concluded that the shape of the model would not change when an additional condition or proposition was added. For instance, in a previous interview question, AM already constructed a mental model of H_2S and answered that the bond angle of H_2S would be smaller than 109.5° because the lone pairs had greater repulsion than the H-S bonds. A new condition – "if we replaced two hydrogen atoms [in H_2S] with two chlorine atoms, how would the bond angle change" was then added to check if AM would adjust her mental model by considering this new condition.

AM started solving the question by drawing a Lewis structure for SCl_2. Once she determined the number of lone pairs and bonding pairs from the Lewis structure, she concluded that the geometry of SCl_2 would be the same as the H_2S. She did not think the bond angle would change "because the sulfate still has…it is still tetrahedral, so the bond angle would be the same as with the hydrogens" (AM, interview). Instead of using the prior mental model of H_2S as a template and modifying it for SCl_2, AM started a new mental model construction. While constructing a new mental model for SCl_2, she neglected to consider the new condition of the problem, that the S–Cl bonds would have greater repulsion between each other and would change the bond angle. SD indicated that the bond angles for SCl_2 and for H_2S would be the same because only changing the numbers of lone pairs and bonds in a molecule could change the bond angle and geometry of the molecule. AM's and SD's cases revealed that they followed a routine to approach a problem and failed to consider the influence of chlorine atoms on the 3D molecular geometry.

After being reminded by the interviewer, AM and SD reconsidered their answers regarding the size of chlorine atoms. They constructed a concrete model incorporating the new information about the size of chlorine atoms, and then adjusted the model to determine how the size of chlorine atoms influences the bond angle. AM misinterpreted the context of the problem, thus she considered the influence of chlorine atom in terms of its electronegativity, rather than its size, which actually has a greater impact to the bond angle. SD held on to her original mental model due to her partial understanding about the VSEPR model. This interaction between mental-modeling ability and the individual's conceptual framework will be discussed later.

Limited or no monitoring for their mental-modeling processes was observed among the MMMA students (Characteristic 3). An absence of metacognition to review the conditions of a problem and to monitor their processes of problem-solving is one possible reason for AM's and SD's possession of a rigid mental model rather than using it as a tool of thinking. For example, AM missed a step of reviewing the influence of the new condition carefully which led to a misinterpretation of the problem. When determining the polarity of BF_3, at one point SD stepped back and critiqued her first mental model which was a T-shape, and proposed a second attempt as a trigonal planar shape. SD justified the second answer: "because…they try and equally space themselves because they do not want to be near each other, because the dispersion force type things. And so they want to be as far away from each other as they can" (SD, interview). SD was aware that her first mental model may have been wrong and generated a new possible answer based on her knowledge about the VSPER model. Due to her lack of understanding about the geometry of trignoal planar, SD could not follow up her metacognitve action to select the correct answer.

Evidence of students' mistakes due to a lack of metacognitive actions may be hard to separate in the excerpts. Yet the absence of monitoring their mental-modeling processes becomes obvious when comparing the MMMA students to the HMMA students.

Also, self-checking their mental models and answers using an alternative approach was not apparent to these students (see Table 21) (Characteristic 4). Students in the MMMA group often did not question the correctness of their mental model. Sometimes these students were uncertain about their answers that were derived from the inferences using their mental model. These students suspected inaccuracies in their mental model, but without further actions to the model once the model was constructed.

CR, for instance, applied the VSEPR model to construct a 3D mental model of BF_3 that contained only partially correct spatial information. He did not realize a flaw in his mental model that the shape of BF_3 was a Y-shape rather than all bonds evenly spaced apart. CR concluded that BF_3 was a polar molecule because in his mental model, the sum of two dipole moments pulling upward was greater than the single dipole moment pulling downward. I then asked him to build a concrete model. Building a concrete model of BF_3 provided CR an opportunity to go through his thinking processes again as an alternative approach to examine the metal model. Based on the VSEPR model, he built the concrete model with a trigonal planar shape and all bond angles were 120°. I probed him to reconsider the difference between spatial information presented by the concrete model and by his mental model. He said:

> CR: But now, I never thought of that before, because, but I mean I never made a model before. But I mean this way [upward] to this way [downward] is essentially equal…same as the same as this way [left] to this way [right], so. Now I think about that, that kind of just another thought in my head, it makes me wonder.
>
> I: So now would you change your answer saying this is polar or nonpolar?
>
> CR: I still think it is polar. Wait, wait, wait, now I think about that, no I do not. I think it is nonpolar now. Because they are all pulling in opposite directions symmetrically and they would cancel out. So I kind of changed my mind at this moment.
>
> I: As you change your answer, do you use the image in your mind, to help you think about it?
>
> CR: Yes I do. Because...see before I was kind of…I forgot that, when I drew it, I drew this one [bond] closer together [bond] and I did not draw it symmetrically, I kind of confused myself and tricked myself into thinking it was polar. But like when you actually do it equally like this and symmetrically have a model in my head, oh they are all pulling the same way. I'm like, wait a second, this [up and down] and that [left and right] is the same span so. [25:43-27:57]

An actual symmetrical concrete model became a useful strategy to provide CR an opportunity to reconsider the balance of dipole moment and to test his unsymmetrical mental model.

Low Mental-Modeling Ability Group (LMMA Group)

Students in the LMMA group constructed a mental model by recalling the geometry of a given molecule algorithmically based on cues such as numbers of lone pairs and bonds in its 2D Lewis structure. Often, these students did not form a mental model (Characteristic 1). Similar to the student SD in the MMMA group, some students in the LMMA group had difficulties visualizing certain molecular geometry. For example, when KA was asked to build a model of BF_3, he built a model with three B-F bonds in a T-shape. He said:

> KA: So they are all single bonds. So it is just the trigonal, right? Like in geometry? This arrangement? I do not have it memorized that well anymore.
> I: Why is it not like this [a right trigonal planar], but looks like a T?
> KA: Unhumm. I think it is bent. It is probably just something I do not really know. Like I know how it looks like… Like if it was tetrahedral, I would not know how it looked like, and if it is octahedral I would not be sure, but I just know that's how a bent looks like. Just like the plane... After it is been bent, it is going to look like it would be even, like a square box or whatever. [14:42-15:06] (KA, interview)

In the excerpts, KA expressed a lack of understanding about tetrahedral and octahedral geometry in 3D. He was also confused by trigonal planar and bent shapes.

While solving problems about molecular shape and polarity, drawing a 2D Lewis dot structure of a given formula was an essential step prior to the LMMA students constructing a mental model. The 2D Lewis structure provided different cues for visualizing a mental model depending on whether a specific molecular geometry was available to recall and to use in an individual's conceptual framework.

When a given molecule had a geometry that the students saw frequently in the textbook or in class, for example, a bent molecule, they used cues, such as numbers of bonding and lone pairs in the Lewis structure, to recall its molecular geometry algorithmically. For instance, after TA drew a 2D Lewis structure of H_2S, he determined that the molecule shape would be bent:

> Because the molecular geometry will show up and that's the rule that it follows… is that if that there are four bonding sides on a central atom and there are two [bonding pairs] that are there and then there are two sections of one, what would be lone pairs. So and that rule, for the molecular geometry would mean that it would be a bent molecule [6:50-7:24] (TA, interview)

Apparently, TA followed a certain rule to determine the molecular shape of H_2S by counting its numbers of lone pairs and bonds. In the following conversation, KA's strategy for dealing with molecular geometry was even more explicit. When KA used play-dough to show the geometry of H_2S, he said:

> KA: I can't remember. Two lone…so it is tetrahedral...two and two...So that's bent, right? It is a bent molecule [for H_2S]?
> I: Yeah. Tell me what just went through your mind?
> KA: Just a graph. I counted up four for...I counted up the total number of lone pairs and bonds and I know four is tetra. So it is going to be a tetrahedral molecule. The geometry… I think I just memorize the geometry. I see two and two and I see bent. That's just my picture in my head. Something like that.
> I: Okay. Tell me more about the details of the pictures in your mind.
> KA: It is like a chart I memorized.
> I: You refer to this one here [in the textbook]?
> KA: Yeah, that one [14:44-16:45].
>
> [He uses a trigonal bipyramidal molecule with five electron pairs as an example to explain his strategy.]
>
> KA: …I pretty much just look at this column [with the number of lone pairs], I think. I know I'm going to have five [electron pairs] anyway. This is the number [of lone pairs] that is important because that's going to tell me if it is seesaw, like one point there; and then like T [shape], the two points [lone pairs] there; and then three [lone pairs] for the linear. [18:18-18:33] (KA, interview)

Earlier, KA indicated that he could not visualize a geometric shape, such as a tetrahedral or other shape, in 3D. So what KA described here was based on algorithmically memorizing 2D representations and word associations for the number of electrons and naming of the geometry, such as "four is tetra" (KA, interview).

Some LMMA students neither understood the underpinning concepts, such as the VSEPR model, nor the rules of thumb to determine molecular geometry. In this case, these students either generated a mental model that had the same shape as the drawing of the 2D Lewis structure, or simply used the drawing of the 2D Lewis structure as a tool for thinking without visualizing a mental model.

Furthermore, their constructed 2D Lewis structures or concrete models did not correct spatial information. For LMMA students, concepts of 3D molecular geometry had only a weak connection or no connections with the VSEPR model in their conceptual framework. They were not aware of which proposition (e.g., the VSEPR theory) they should apply, why they should apply it, and what it would do to the model. For example, JT mistakenly applied propositions of electronegativity difference and bond polarity to a 2D, linear, Lewis structure on paper. He determined that the geometry of H_2S is linear because the bonds on each side canceled each other and the lone pairs on each side also canceled each other. Similarly, KA and TA referred to the geometry of BF_3 as T-shape; although they both were uncertain about their answers. This insufficient understanding may be due to a lack of multiple types of prerequisite knowledge, which will be discussed in Chapter Five.

The LMMA students preferred to draw a 2D Lewis dot structure on paper as a tool of thinking and then apply propositions or conditions of a problem to the 2D Lewis dot *structure for inference (Characteristic 2).* Instead of generating a mental model and using it as a tool for thinking, the LMMA students preferred to draw out a 2D Lewis dot structure and then apply propositions manually on paper. TA indicated that, "I usually, just drawing things out better, it helps me out more than, like, putting it in my head and thinking" (TA, interview). Instead of thinking in their mind about how the difference of electronegativity between two atoms influenced the electron cloud distribution, the LMMA students drew arrows along the bonds on paper pointing from less electronegative to the more electronegative atoms. I use KA's case to demonstrate his inference about H_2S polarity based on a 2D Lewis structure on paper:

> I: Would you say hydrogen sulfide is a polar or nonpolar molecule?
> KA: It would be polar…Because of its geometry. I know that since sulfur is more electronegative it'd be…I know that there would be a dipole moment in this direction [on one S-H bond], and a dipole moment in this direction [on the other S-H bond].
> I: Why did you draw in that direction?
> KA: I really do not know why. It is what one of my tutors said to do. He said that since sulfur is more electronegative you just draw the arrow in that direction and draw the tail.
> I: Pointing toward the one that is more electronegative? Okay.
> KA: Uh, huh. So it is polar. That's the net total. I think that's the way it would pull. [5:04-6:10]

LMMA students, who reasoned and inferred based on their drawings of 2D Lewis structures, were mentally disadvantaged by the rigid structure and inaccurate spatial information of the drawings. Unless it is redrawn, the 2D Lewis structure permits less flexibility and adjustability for students to modify the model accordingly when an additional proposition or condition was imposed. Reasoning based on 2D Lewis structures, LMMA students often derived wrong conclusions due to the incorrect spatial information of the 2D Lewis structure.

After constructing a mental model and using it as a thinking tool, a LMMA student was able to infer a correct conclusion by adjusting the shape of the concrete molecule while applying a proposition to the model. For example, TA drew the Lewis structure of BF_3 in a T-shape on the paper. He applied the notion of electronegativity difference to each B-F bond on the 2D Lewis structure and concluded that BF_3 was a polar molecule because "these two would cancel each other out, and then there's nothing up here for the fluorine to pull against, so it would pull the whole molecule downward" (TA, interview). When TA was asked to construct a concrete model, he first built the model in a trigonal pyramidal shape and then switched to a T-shape. When I asked again about if he still thought that BF_3 is a polar molecule, he answered:

> TA: I would still think so because…regardless if it is in a plane or if it is a pyramid that these are still pulling and it is just leaving that there but… because this is pulling it down… I think that yeah, that would I think be its…[He spoke while adjusting the 3D molecule from a T-shape to a trigonal planar]
>
> TA: Wait, then it would not be polar, it'd be set up like that…
>
> I: Why do you say that?
>
> TA: Because now they all have equal distance around each other, and they'd all be pulling their own way. This way [the T-shape] these two would just cancel each other out and they'd be left with this one. But this way [the trigonal planar] all three are…I'd probably say they'd go like this and it'd be a non-polar. [18:36-18:20]

TA applied the notion of electronegativity difference to the concrete model and thought that one force would be left pulling downward after the other two forces would cancel each other. While he was pulling the bond on the concrete model, the shape of the model was changed from a T-shape to a right trigonal planar shape. The new shape triggered TA to reconsider the balance of forces among three B-F bonds and changed his answer about polarity of BF_3 to nonpolar.

The LMMA students did not monitor their processes of mental modeling. At the end of the inference or reasoning, these students did not perform self-checking to test or inspect mental models or 2D representations using an alternative approach (Characteristics 3&4). While solving a problem, each LMMA student in this group made errors. TA, for instance, added the number of valence electrons incorrectly; thus he considered H_2S as an exception to the octet rule with only seven valence electrons (TA, interview). After drawing directions of bond polarity for H_2S with the hydrogen atom toward the sulfur atom, KA thoughtlessly applied the same directions to sulfur dichloride, thinking the direction of bond polarity was from the chlorine atom toward the sulfur atom. Without reviewing the condition of the problem carefully (e.g. the difference of electronegativity difference between S-Cl and S-H bond), KA neglected that chlorine atoms had greater electronegativity and the directions of bond polarity should be toward the opposite direction (KA, interview). Both TA and KA were not aware of their mistakes unless noted by the interviewer. Observations of these interviews indicated that neither self-checking to identify errors from the 2D representations nor monitoring modeling process occurred.

Levels of Content Knowledge about Molecular Geometry, Polarity, and Prerequisite Concepts

In this section, three conceptual frameworks: (1) atomic structure, periodic trends, and representations of atomic models, (2) chemical bonding and the octet rule, and (3) molecular shape and molecular polarity were used to organize characteristics about students' content knowledge into high, moderate, low content knowledge groups (Table 20). For each conceptual framework, a concept web was developed to provide a visual representation for comparing similarities and differences across the high, moderate, and low student groups. These three concept webs include ten clusters of concepts associated with molecular geometry, polarity, and prerequisite concepts (see Table 5). In the following sections, I discuss the content and quality of students' conceptual frameworks content knowledge for the high, moderate, and low content knowledge groups. At the end of this section, a table is presented to organize the cross-case comparisons.

Conceptual Frameworks for Students with High Content Knowledge (refer to JS's, RE's, and CR's concept webs, Figure 6-14)

I categorized JS, RE, and CR as students who possess high content knowledge about molecular geometry, polarity, and prerequisite concepts. In this section, I describe concepts and the structure of conceptual frameworks of students in the high content knowledge group and their misconceptions as well. Evidence from these three students' interview responses and misconceptions identified from the diagnostic instruments will be used to support the descriptions.

Atomic structure, periodic trends, and representations of atomic model (refer to JS's, RE's, and CR's concept webs of atomic model). Descriptions about atomic structure for students in the high content knowledge group were characterized with detailed features. When JS and RE described a fluorine atom and a chlorine atom, they both portrayed the atoms using a Bohr model with a nucleus composed of protons and neutrons and electrons filling electron shells (Figure 15). JS, RE, and CR never explicitly indicated the influence of effective core charge to the nucleus-electrons interaction, and only JS used the term "electrostatic force" to describe the attraction between the nucleus

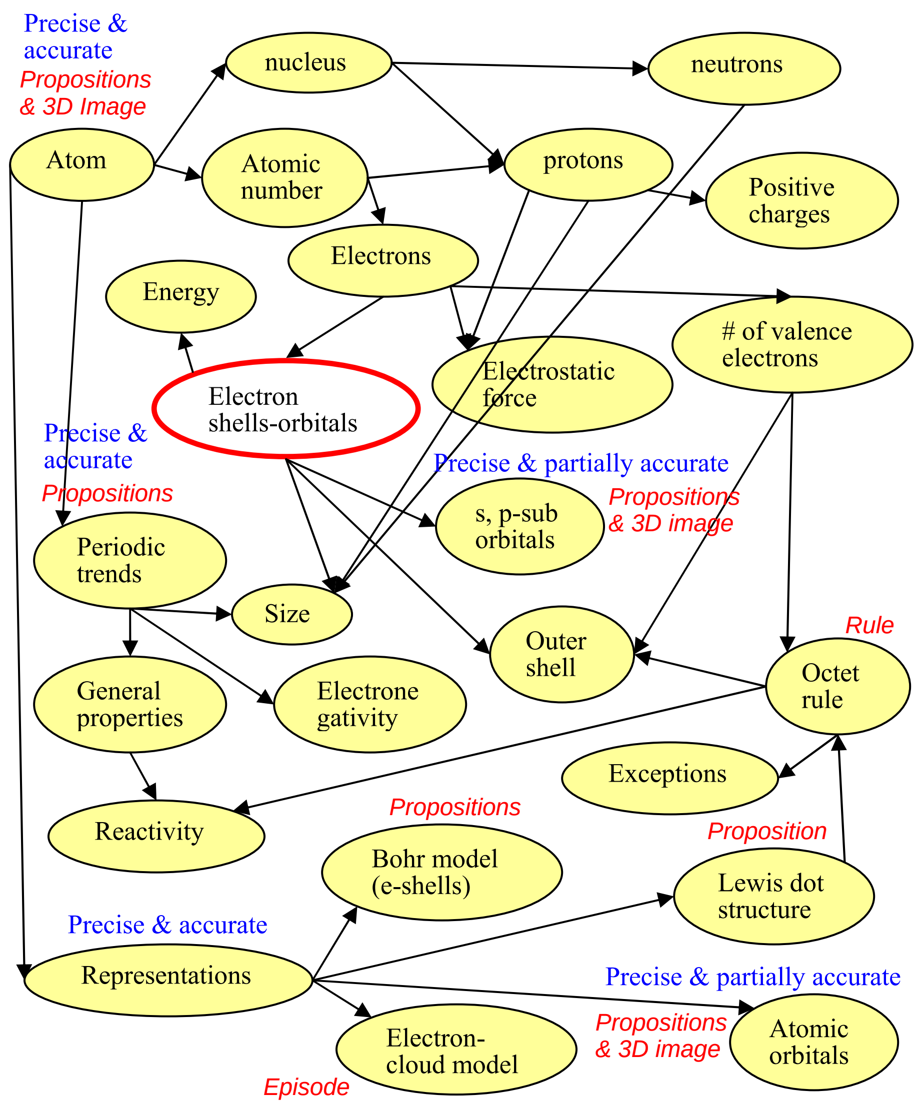


Figure 6. JS's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

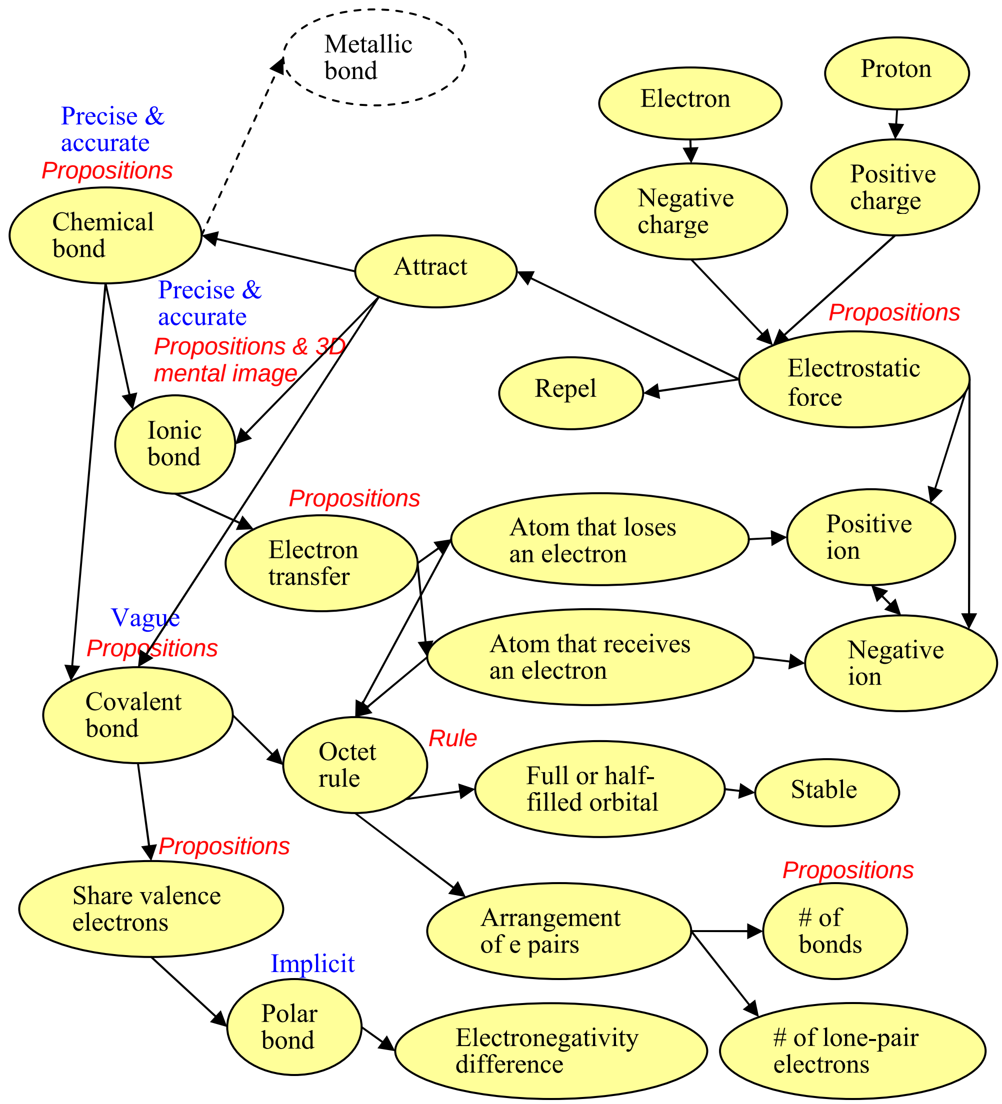


Figure 7. JS's concept web on chemical bonding.

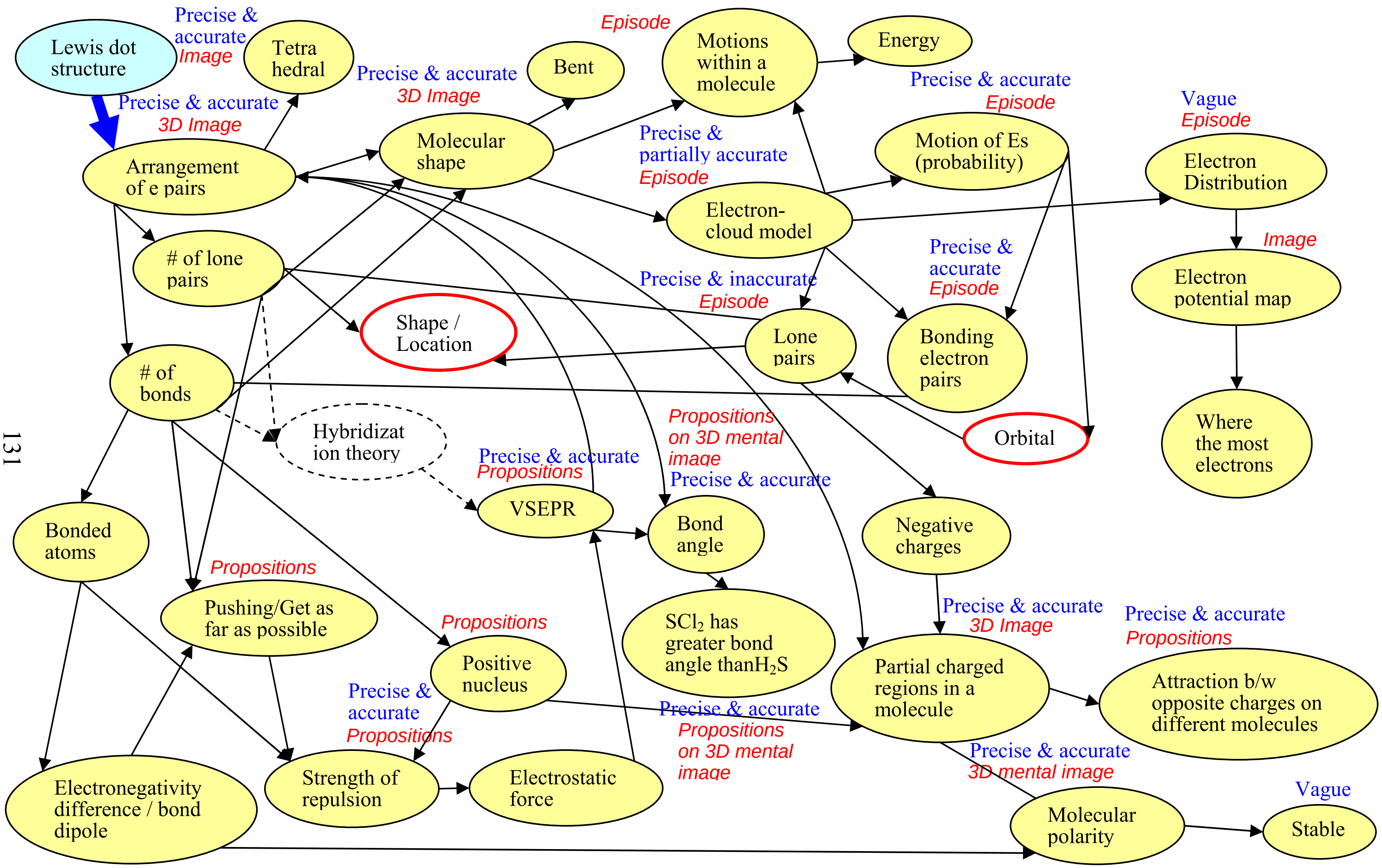


Figure 8. JS's concept web on molecular geometry and polarity.

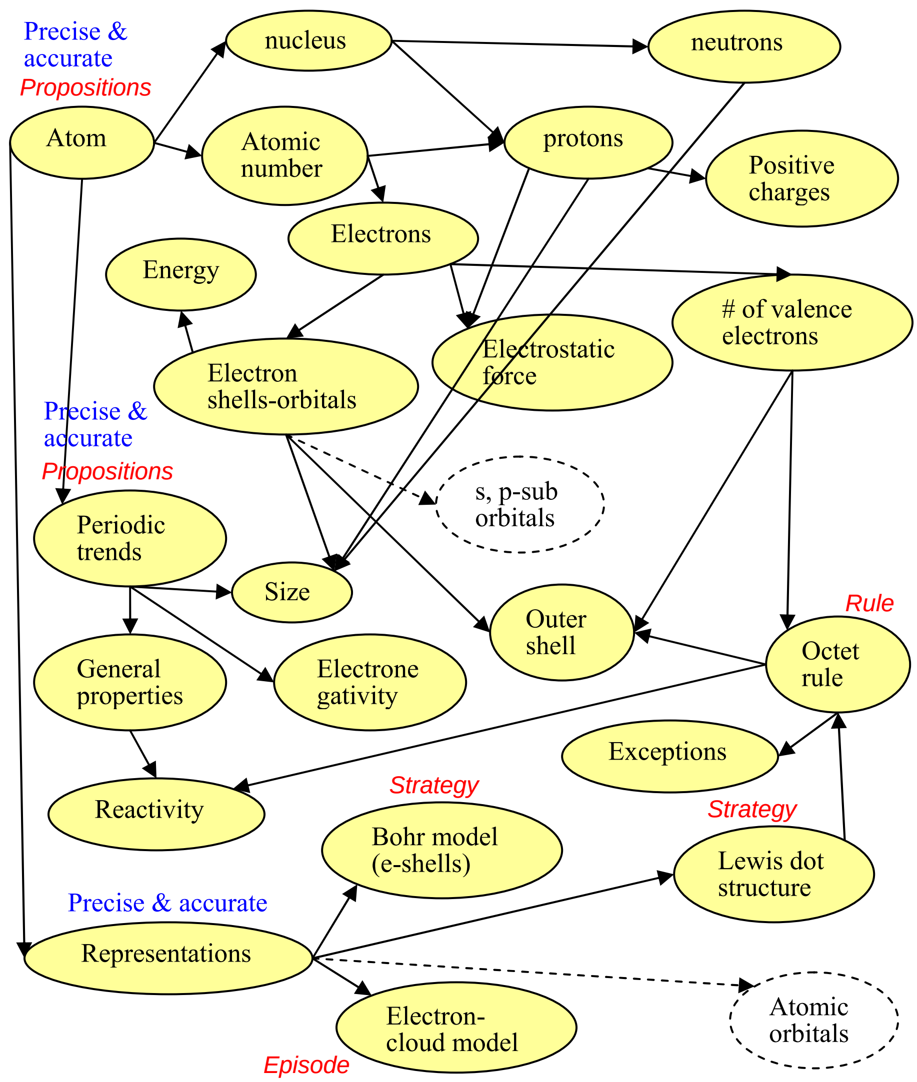


Figure 9. RE's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

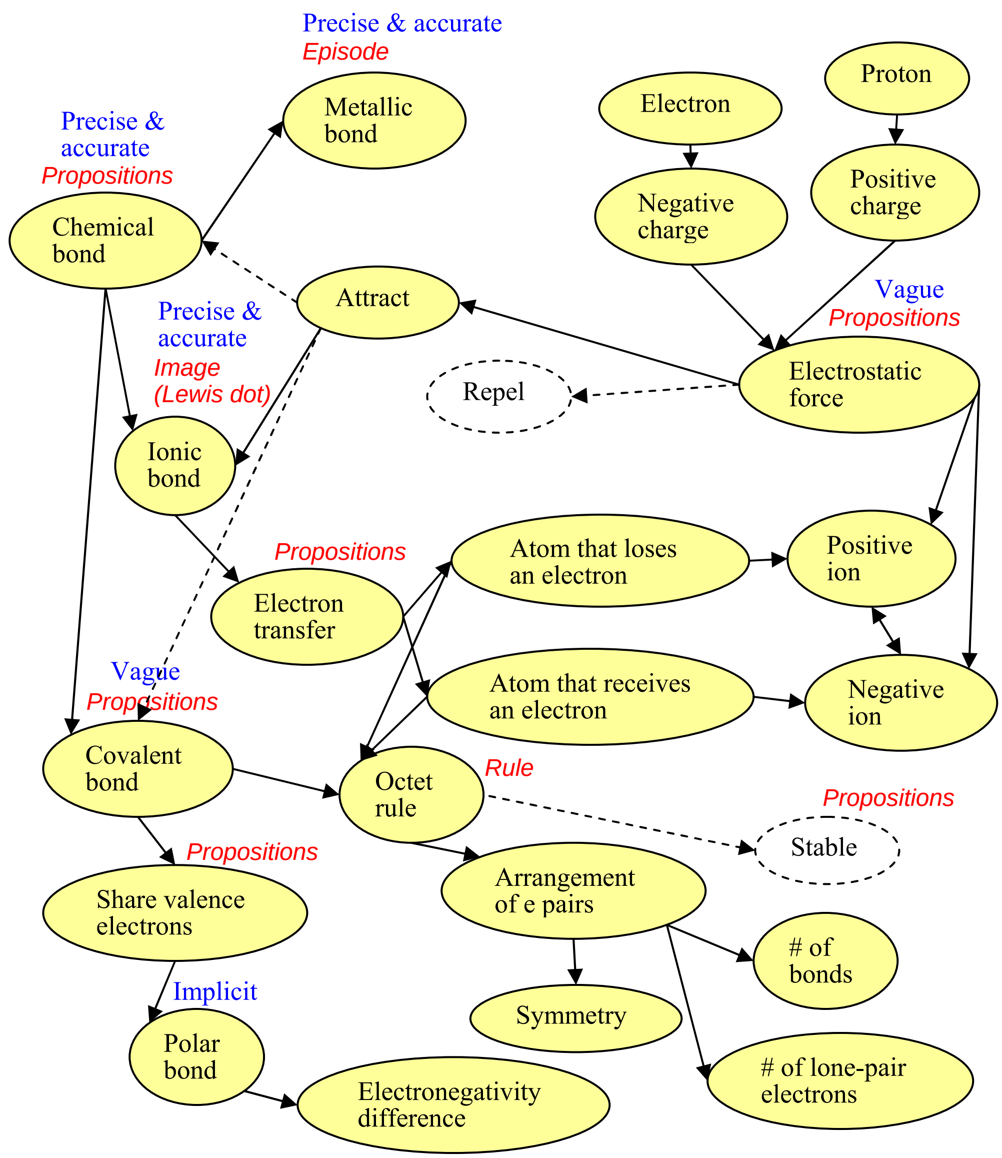


Figure 10. RE's concept web on chemical bonding.

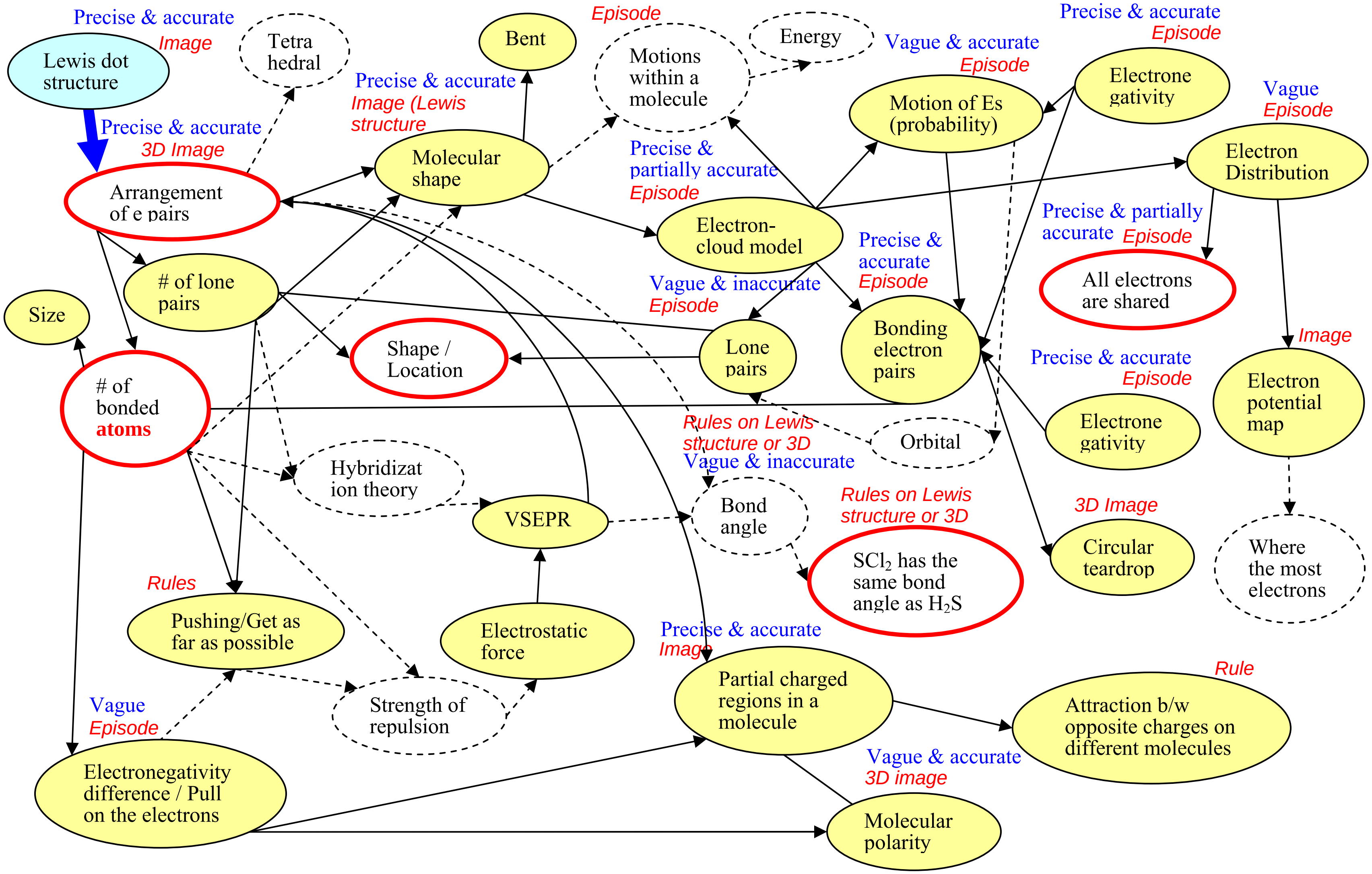


Figure 11. RE's concept web on molecular geometry and polarity.

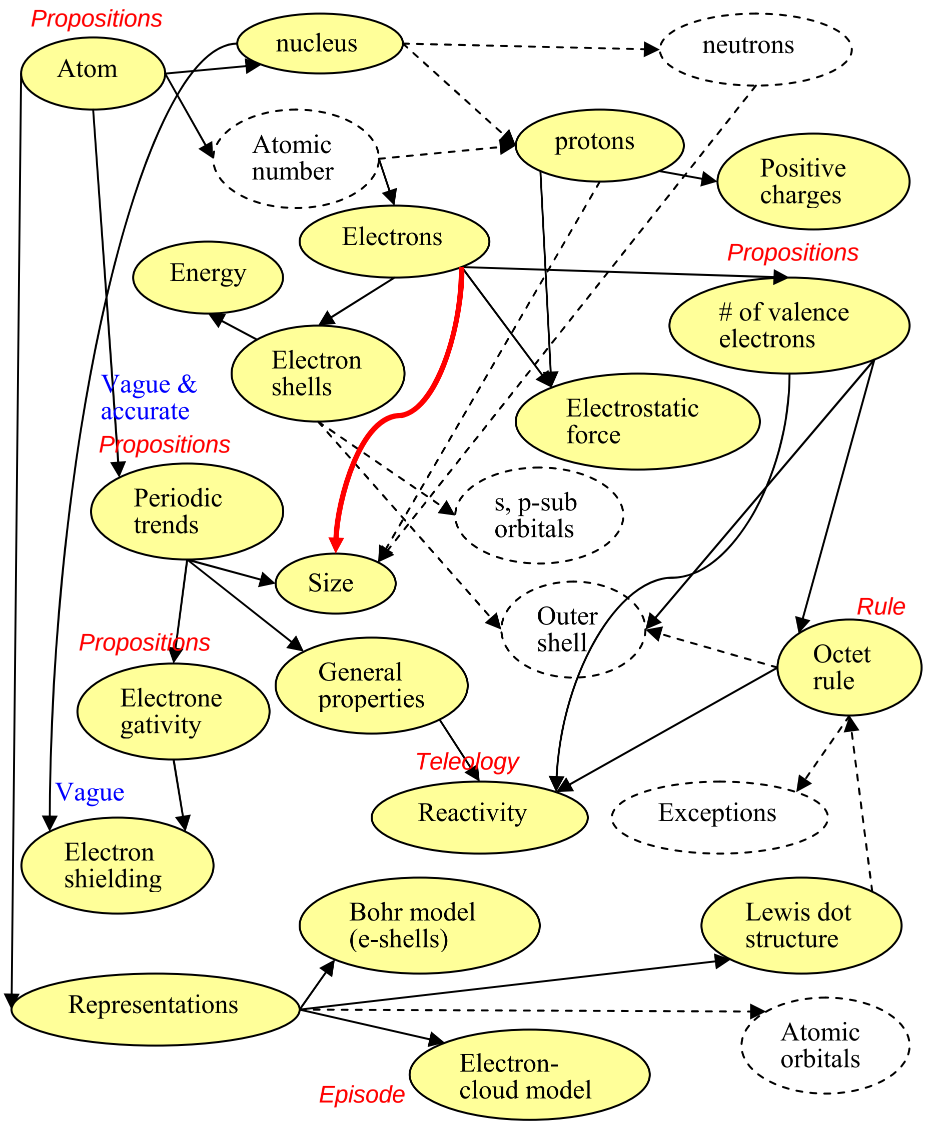


Figure 12. CR's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

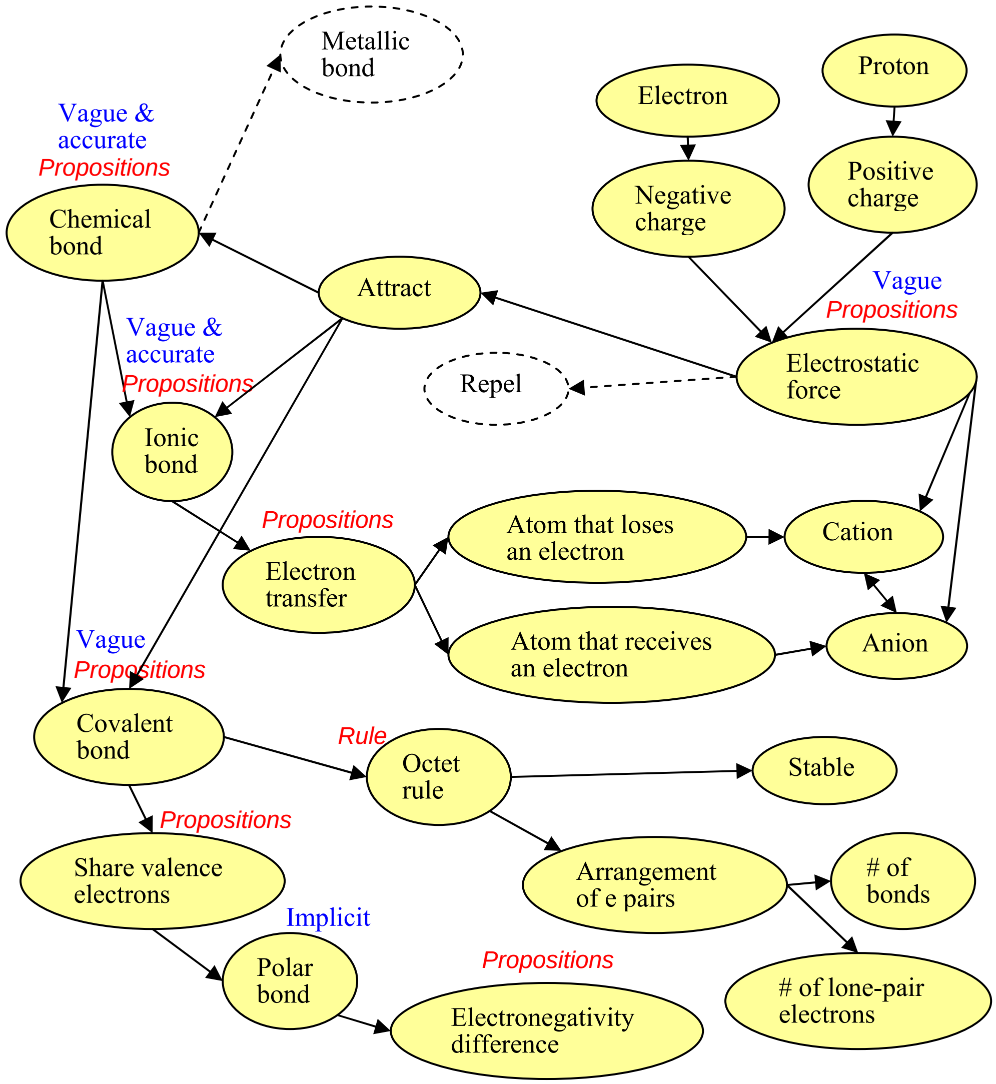


Figure 13. CR's concept web on chemical bonding.

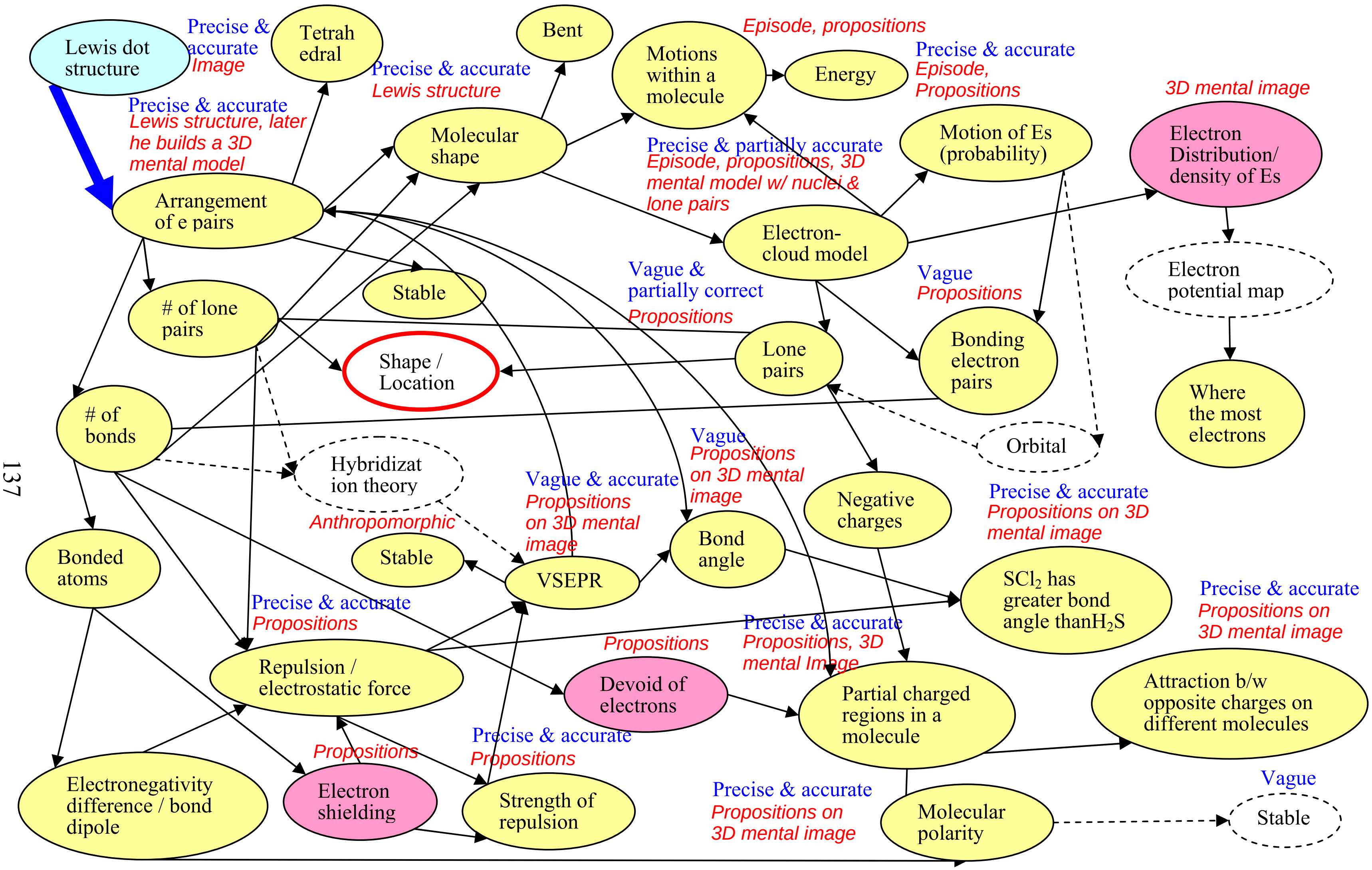


Figure 14. CR's concept web on molecular geometry and polarity.

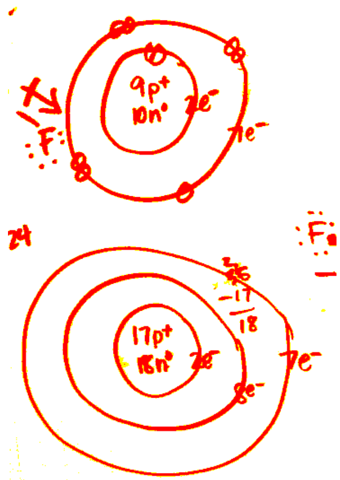


Figure 15. RE’s drawings of a fluorine atom and a chlorine atom.

and electrons in an atom. These three students were aware that “nucleus is attracted to the electrons,” “energy is required to remove an electron from the atom,” and “electrons in the inner electron shell requires more energy to remove because it is in a lower energy level” (EN-5, 1, & 9). Their responses to the instrument EN showed that these students understood the existence of attractive force between the positive nucleus and negative electrons, and the layers of electron shells involved different energy levels.

Students in the high content knowledge group closely tied their understanding about atomic structure to concepts of periodic trends. These students used the Periodic Table as a summary table for characteristics of atoms. For example, JS and RE were able to use the Periodic Table correctly to describe a fluorine atom’s and a chlorine atom’s atomic number, numbers of protons and neutrons in the nucleus, and accurate numbers of overall electrons and valence electrons on the electron shells. Also, all three students could compare relative strength of electronegativity and atomic radius for hydrogen, fluorine, chlorine, and sulfur based on the position of these atoms in the Periodic Table.

These students used their understanding about atomic structure to conceptualize periodic trends such as atomic radius. For example, JS and RE associated a trend of atomic radius in the halogen group to the increase in the numbers of protons, neutrons, and electrons. "Atoms in the same group of the Periodic Table have similar chemical properties, such as electronegativty and reactivity" was mentioned by these three students. CR correctly explained electronegativity of an atom in terms of the strength of attraction between the nucleus and electrons in an atom. He could also relate the strong electronegativity of a fluorine atom to its less shielding effect while comparing it with other atoms in the halogen group.

The octet rule was an underpinning idea when RE and CR described "highly reactive" as a similar characteristic for a fluorine atom and a chlorine atom. RE and CR both considered that a fluorine atom and a chlorine atom react very similarly because of their tendency of "getting one valence electron" (CR, interview) to fill the outer shell. RE attributed the reactivity of a fluorine atom and a chlorine atom to the same reason saying:

> They [fluorine and chlorine atoms] have pretty much the same general properties because….like say you have a sodium ion, it is gonna really easily react with either one of these [fluorine and chlorine] because it is got one valence electron and both of these have seven so…to get that eight in the outer shell, it is gonna really easily react [03:37-04:34] (RE, interview).

To RE and CR, removing a valence electron or wanting one more valence electron to have "eight" electrons in the outer shell becomes a driving force to justify the strong reactivity for alkali metals and the halogen group.

Although all three students with high content knowledge, they preferred using the Bohr model when they drew and explained about atomic structure. Also, they visualized an atom in three dimensions with an electron-cloud surrounding the nucleus (RE and CR, interview) or like a ball with layers of concentric orbitals (JS, interview). Also, JS, RE, and CR were all able to describe their idea of electron-cloud model with quantum mechanics descriptions.

Chemical bonding and the octet rule (refer to JS's, RE's, and CR's concept webs of chemical bonding). Two propositions, electrostatic force and the octet rule, seemed to underpin JS's, RE's, and CR's thinking about chemical bonding. These three students applied their understanding about electrostatic force between a positive nucleus and negative electrons in an atom to conceptualize the concept of chemical bonding as attractions of electrostatic force between two atoms. JS's explanations about chemical bonding provided a good example. He said:

> I think of covalent and ionic bonds, and just how the electrons are negative and the protons are positive and how those attract and repel, but I guess with bonding we're going to have to talk about how they attract, how the electrons and the protons attract each other. (JS, interview)

When JS, RE, and CR reconciled this concept about chemical bonding as electrostatic force with the ideas of electron-sharing as covalent bonding or electron-transferring as ionic bonding, an underlying presupposition about "atoms want to fulfill the octet rule" was used to justify the formation of ions. The electrostatic force was then attributed to the attractions between cations and anions. For instance, when CR was asked to give an example about chemical bonding, he said:

> I'm thinking of sodium has the one electron that it wants to get rid of and then chlorine has one of these [electrons] to gain. So chlorine kind of brought this one [electron], but then they'd be held together by that. (CR, interview)

JS's and RE's explanations followed the same line and implied that ionic bonding is electron-transfer where:

> [Electrons] can be given up to make a complete orbital that, I guess, is more stable and at the same time creating maybe ions that one would be negative,

> one would be positive, and that's the reason that they bond because the difference in charges. (JS, interview)

The underpinning presupposition about the octet rule was evident by these three students' responses to instrument EN. They justified the octet rule with an alternative notion of stability. On one hand, they thought that a sodium atom would be more stable if it "lost an electron" (EN-18) or "gained seven electrons" (EN-20). While RE and JS had correct understanding about "energy is required to remove an electron from the atom" (EN-1); thus "the atom will not spontaneously lose an electron to become stable" (EN-3). They also rejected the statement about "if the outermost electron is removed from the [sodium] atom it will not return because there will be a stable electron configuration" (EN-12). RE and JS were neither aware of, nor reconciled these two conflicting ideas. In CR's case, the octet rule was an underlying presupposition that he consistently applied through out these items.

JS, RE, and CR extended this notion of the octet rule to explain formations of covalent bonds and a covalent compound when drawing a Lewis structure. For these three students, forming a bond and drawing a Lewis structure of a given chemical formula was to find a way to share or give up valence electrons from each of the atoms to achieve noble gas electron configuration to be stable. In other words, atoms form chemical bonds or a chemical compound in order to achieve its octet or to have eight electrons. For example, when JS explained his thinking processes when drawing a Lewis structure for hydrogen sulfate (H_2S), he said:

> You have to understand that whenever you're bonding you want a complete orbital, so you want to achieve either a), which is this last row [of the periodic table] or, in the case of hydrogen and helium... So if you're wanting to get eight [electrons], you have to find a way to share or give up electrons

> from each of these [atoms] to make it so that each orbital is as complete as it can be, or is completed. (JS, interview)

CR's explanations were similar to JS's:

> First, I would just explain that for each atom to be stable they want to have an octet. So sulfur if you look at the periodic chart, it has six valence electrons. So in order to have an octet you need two [valence electrons], and each hydrogen has one valence electron. In order for everyone to be happy, you would need two hydrogens to satisfy the sulfur. [4:53-5:16] (CR, interview)

CR used a few terms such as "happy" and "satisfy" which were commonly recognized as alternative conceptions in chemical education literature (Taber, 1998). But analyses of his concept webs showed that CR possessed a coherent and scientific understanding about principles of electrostatic force with concepts about atomic model and chemical bonding. Thus he may simply use "happy" and "satisfy" as metaphoric terms.

Molecular shape and molecular polarity (refer to JS's, RE's, and CR's concept webs of molecular shape and polarity). For students in the high content knowledge group, their procedures to determine geometry and polarity of a molecule can be summarized by two steps: (1) apply a VSEPR model to determine the arrangement of electron pairs in 3D; and (2) apply a proposition about electronegativity difference to the 3D molecular structure that determine the directions of "pulling of electrons" (only CR used the term "dipole moment") for each bond; and cancel the "pulling of electrons" spatially and determine the molecular polarity. These two steps were divided based on students' logical thinking processes for the purpose of comparison in order to describe the distinction among students in the high, moderate, and low content knowledge groups. During the interviews, these three steps took place in seconds in students' mind.

Step 1. All students with high content knowledge drew a correct Lewis dot structure with accurate numbers of lone pairs and bonding pairs for a H_2S molecule. They had no difficulty with drawing a Lewis structure of BF_3 and were comfortable about treating BF_3 as an exception of the octet rule. Although none of the three students used the term "VSEPR model" during the entire interview, their explanations captured the main ideas from the VSEPR model. JS, RE, and CR were able to apply a notion of repulsion between electron pairs to reposition electron pairs of a Lewis structure and determine its molecular shape. They also justified the source of repulsion with an electrostatic force between electron pairs and indicated that lone pairs have greater repulsion than bonding pairs. The conversations between the interviewer and CR illustrated his thinking processes to determine the molecular shape of H_2S:

> CR: Well since you have these two, these four lone pairs of electrons, then it would make it a bent, a bent shape instead of purely linear.
> I: Why?
> CR: Because the electrostatic, the repulsion between lone pairs, and it is greater than that between bonding pairs.
> I: Okay, so as you're describing this to me, do you have an image in your mind that helps you think through those?
> CR: Well, first when I'm trying to figure out the geometry of a particular molecule what it might look like, first off I rely on, I think of an actual position of electrons even though that's not how it really is, even though it is a probability cloud. But I just keep in the back of my mind that it is, that they can be anywhere in probability. But knowing, but I use this model [Lewis dot structure] to kind of help me get the initial geometry. [9:41-10:13] (CR, interview)

In students' descriptions about molecular geometry, I found that their notions about lone pairs as a feature of the mental model for a H_2S molecule were different and influenced their determination of the bond angle of H_2S. For example, CR conceptualized the two lone pairs of H_2S as four overlapped spheres that each represented a region of density for a lone pair electron. RE represented the two lone pairs of H_2S as two sets of two dots when she built a concrete model. But she described that all the lone pair electrons:

> Are being shared, like just kind of around that area and they're all kind of going to be mixed together. Like…But I do not think it would be as distinct, like it is not going to be: here's this lone pair, here's this lone pair, you know. It is going to be more like all mixed together. [18:08-18:57] (RE, interview)

Both CR's and RE's mental models for H_2S were not a tetrahedral shape and did not contain correct spatial information due to their alternative idea about lone pairs. Therefore, CR and RE were not able to predict the bond angle of H_2S. After the interviewer gave a hint by asking "do you think the lone pairs will be in a planar shape or a tetrahedral shape with the two S-H bonds," both CR and RE were able to reconsider their mental models and decided that the arrangement of electron pairs should be tetrahedral. They also reconciled this new mental model with their existing knowledge. I used RE's case to demonstrate this process of reconciliation:

> I: So do you think that these two pairs of nonbonded electrons will be here [as planar] or be here [as tetrahedral]?
>
> RE: Um…well…I…I guess they could be here, I mean I guess I never really thought of it that way because mostly what I picture is like the Lewis structures. So actually I never thought of them being there. So, I mean, yeah, I guess it would make sense that they can be there because that puts everything a little bit further apart and actually I guess if I think to how like, the shape of the…where the electrons are would be tetrahedral. And then because you have the two lone pairs it becomes bent. If it was tetrahedral and these were atoms, these would be here. So I guess that would make sense [12:52-13:57].

Step 2. Students in the high content knowledge group used the term "pulling the electrons away" (RE, interview) from a less electronegative atom to a more electronegative atom while explaining bond polarity. Also, they were able to construct a mental model of electron-cloud and applied quantum mechanics descriptions to the model to conceptualize concepts about bond polarity and the polar molecule. Their mental model was functional, allowing the individual who constructed it to apply a proposition of electronegativity difference to manipulate the electron cloud. These students visualized an uneven distribution of electrons around a more electronegative atom and a less electronegative atom as the result of mental modeling. RE visualized a polar bond as "electrons almost like bouncing back and forth between the two nuclei and like spending more time at the more electronegative atom but just kind of like floating back and forth between the two [nuclei]" (RE, interview).

All three students described a polar molecule as a molecule that has a part that is more negative and the other part is more positive. For example, to determine whether H_2S is a polar or nonpolar molecule, CR constructed a mental model using a electro cloud model and visualized the distribution of electron density to illustrate regions of electron-rich and electron-devoid in his mind. He described his mental model:

> …you have the region where there's lots of negative charge. You got a dipole moment from this negative charge going from these lone pairs, and because this area over here [around hydrogen atoms] is like in a sense devoid of electrons, like there's not that many electrons there. There's not as much probability of electrons being there I suppose you'd say. So this is going to have an overall more negative charge over here [around sulfur atom], making it polar. [15:42-16:35] (CR, interview)

After identifying which atoms were more electronegative and which were less, students determined bond polarities and molecular polarity almost simultaneously. Here I use RE's case as an example. Requested by the interviewer, RE described her thinking processes about how she determined BF_3 as a nonpolar molecule. She applied the VSEPR model to conclude that the four atoms should be on the same plane in a triangular shape because there was no lone pair and three bonding pairs wanted to stay away from each other. She then inspected her mental model based on the presupposition that these three bonds should be evenly spaced apart. Based on this mental model, RE determined a direction of dipole moment (in her word, "pulls") for each bond spatially based on electronegativity of the atoms and mentally balanced the directions and strengths of the forces applied on the model:

> And then I said, okay, then if I had these three and they're going to be evenly spaced apart…the angles are all going to be the same then the pulls are going to be towards the fluorines and it is going to pull, like one's pulling this way, one's pulling this way, one's pulling this way. And it is going to cancel, they're all going to cancel out. (RE, interview)

While RE explained her thinking processes, her hands were gesturing in the air, placing one boron and three fluorine atoms in a trigonal planar and showing the directions of the "pulls" on the imaginary molecule. Being a HMMA student, RE's mental-modeling ability allowed her to form a mental model as a thinking tool and to apply concepts to the model effectively for reasoning.

General descriptions about conceptual frameworks. Based on the construction and analysis of concept webs and observations of their interviews, students with high content knowledge possessed key concepts in the three conceptual frameworks. Their descriptions of most of the concepts were precise and accurate. These students had relatively fewer misconceptions and missing concepts and assimilated and reconciled new information using existing knowledge consistently. Thus, the links between/among concepts were correct and coherent while explaining a concept or a phenomenon. These students also justified their explanations with appropriate concepts, rather than merely following rules of thumb.

Students with high content knowledge possessed better understanding about different representations (e.g., space-filling, balls-and-sticks models, and Lewis structure) and models (e.g., Bohr model, electron-cloud model, and quantum mechanics descriptions). Also, they tried to connect and reconcile these models and representations. I use RE's case to demonstrate how a high content knowledge student reconciled her knowledge about two models. When RE described her electron cloud model, she said:

> You have your molecule and you have the nuclei that the electrons are just kind of like in the cloud around them…you can see where would be more electrons or less electrons, but it is not like where this electron always is or something like that…because it [electrons] would be moving all around so it'd be hard to catch it unless you took a picture I guess. [19:04-19:56] (RE, interview)

RE first described the electrons as a cloud surrounding the nuclei in a molecule with an uneven distribution. She further clarified that the electron cloud was not composed of static electrons, rather she used the metaphor, "It'd be hard to catch it unless you took a picture" to explain quantum mechanics descriptions.

Due to the reconciliation of understanding about models and representations, these students were able to switch between models and representations with minimal difficulties. These models also were functional for explanations and problem-solving. Based on the students' understanding about the meanings, explanatory powers, and limitations of the models and representations, the high content knowledge students were able to identify the problems and to choose an appropriate model or representation accordingly.

Conceptual Frameworks for Students with Moderate Content Knowledge (refer to AM's and SD's concept webs, Figure 16-21)

SD and AM belonged to the group of students who demonstrated moderate content knowledge about molecular geometry, polarity, and prerequisite concepts. Based on her scores on the three diagnostic instruments, AM was originally categorized as a low-scoring student. Results of AM's interview and her concept webs analyses indicated that she possessed more prerequisite concepts and fewer misconceptions compared with her cohorts in the low content knowledge group. Thus AM was relocated to the moderate content knowledge group.

In this section, I describe concepts and structures of conceptual frameworks for students in the moderate content knowledge group. Evidence from SD's and AM's interviews and misconceptions identified from the diagnostic instruments are used to support my descriptions.

Atomic structure, periodic trends, and representations of atomic model (refer to AM's and SD's concept webs about atomic model). Students in this group described atomic structure with less detail compared with students in the high content knowledge group. AM and SD both drew a Bohr model while describing a fluorine atom and a chlorine atom. Features of their Bohr model were mainly associated with electrons, and details about the nucleus were missing from their drawing. When AM drew a Bohr model for a fluorine atom, she described:

> The center are the nucleus and then the first ring. Just two electrons because that's all it could hold. And the outer ring has seven valance electrons. And I put nine [beside the Bohr model] because it has nine electrons all together. That's all I would draw. [2:52] (AM, interview)

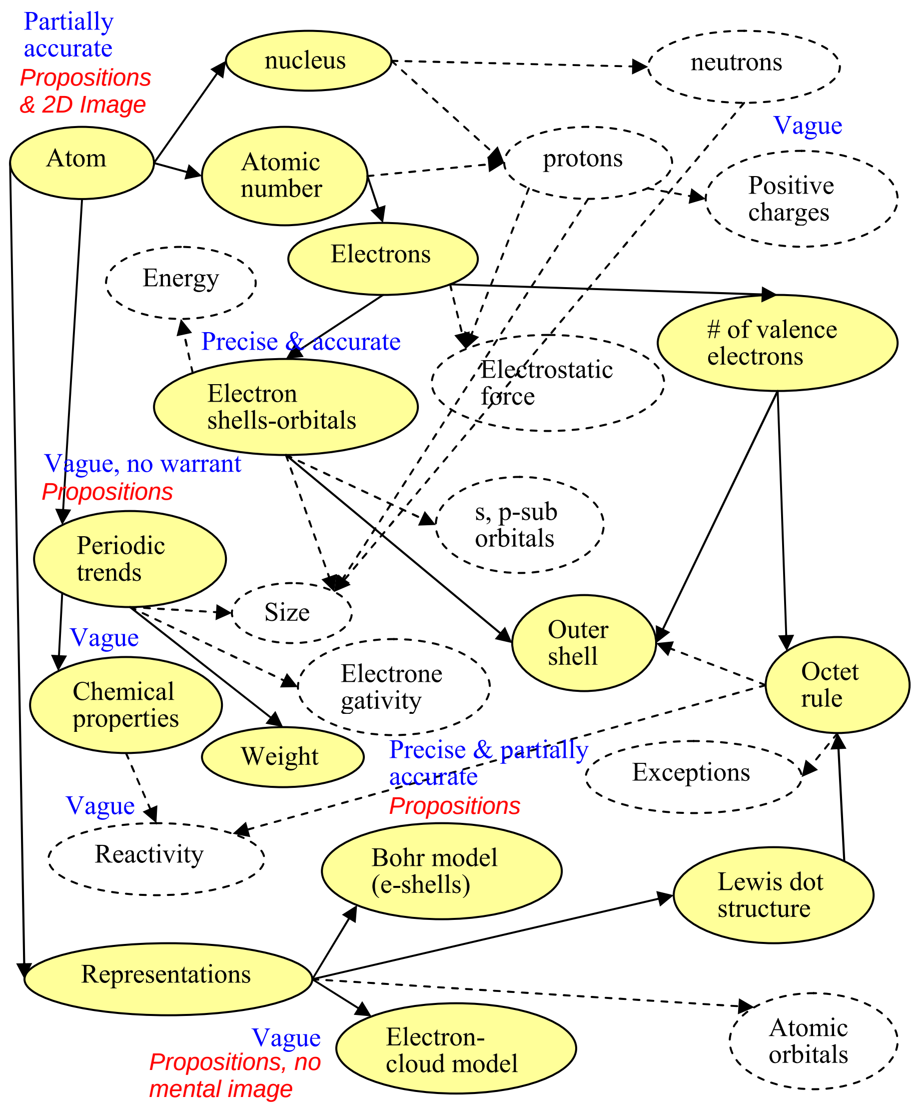


Figure 16. AM's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

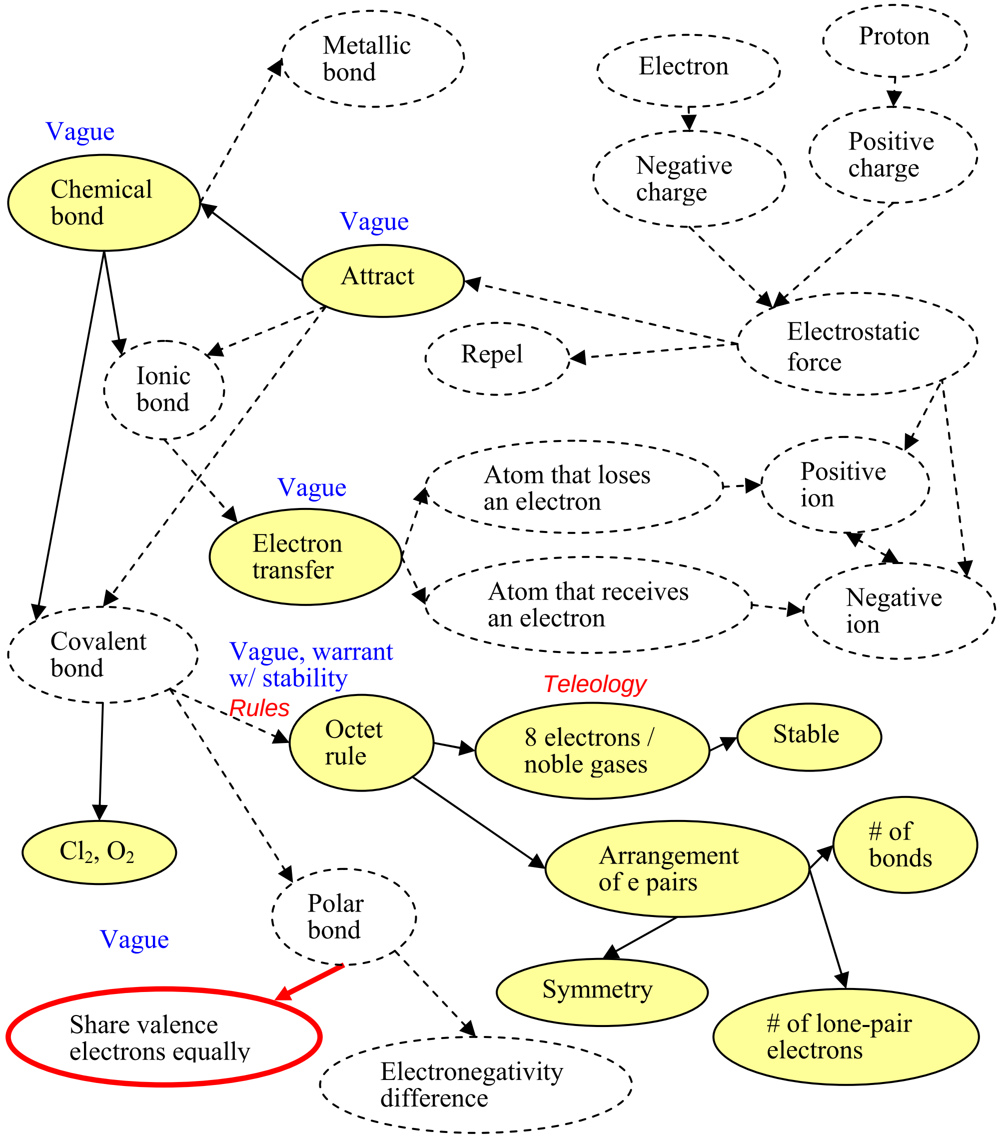


Figure 17. AM's concept web on chemical bonding.

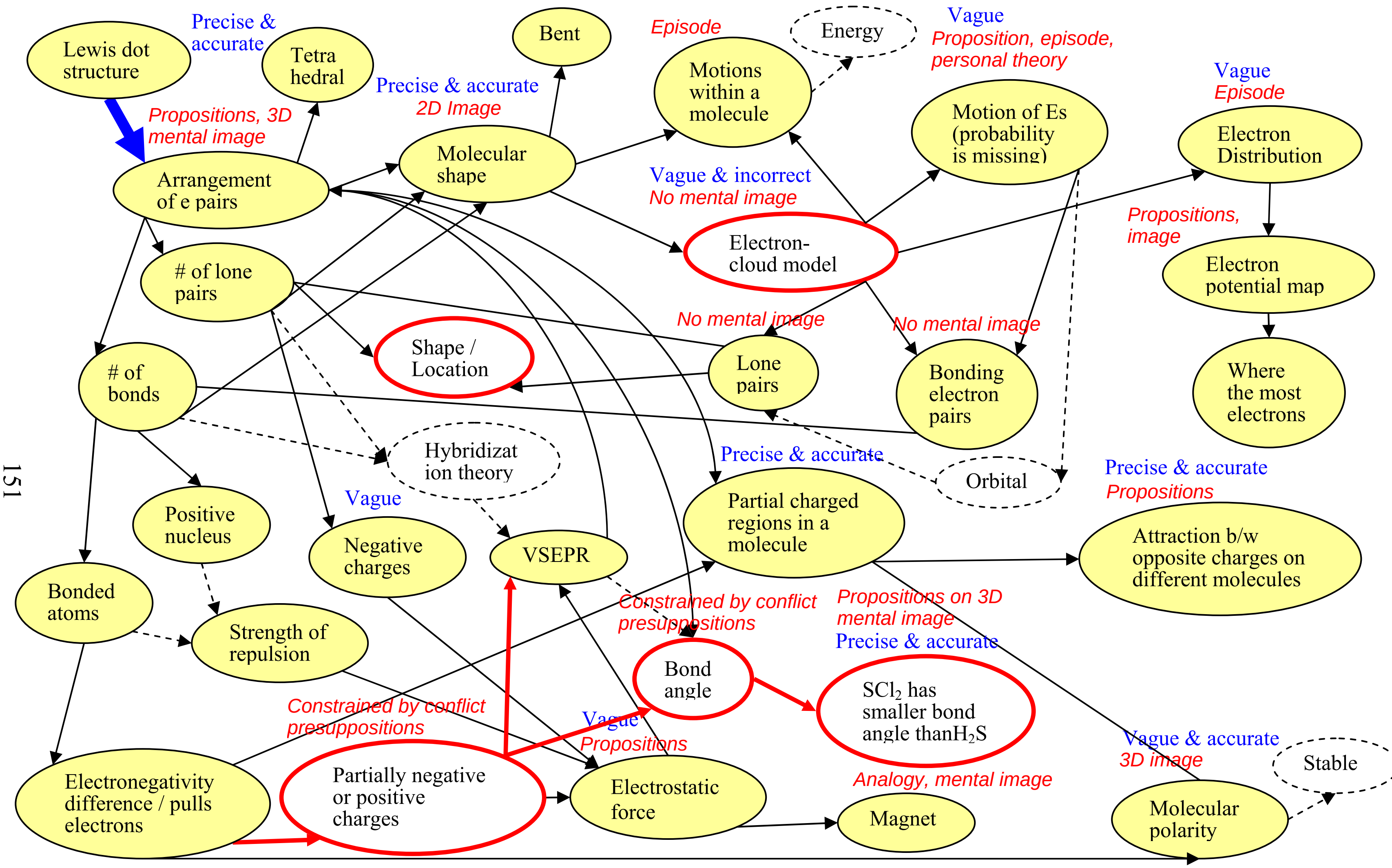


Figure 18. AM’s concept web on molecular geometry and polarity.

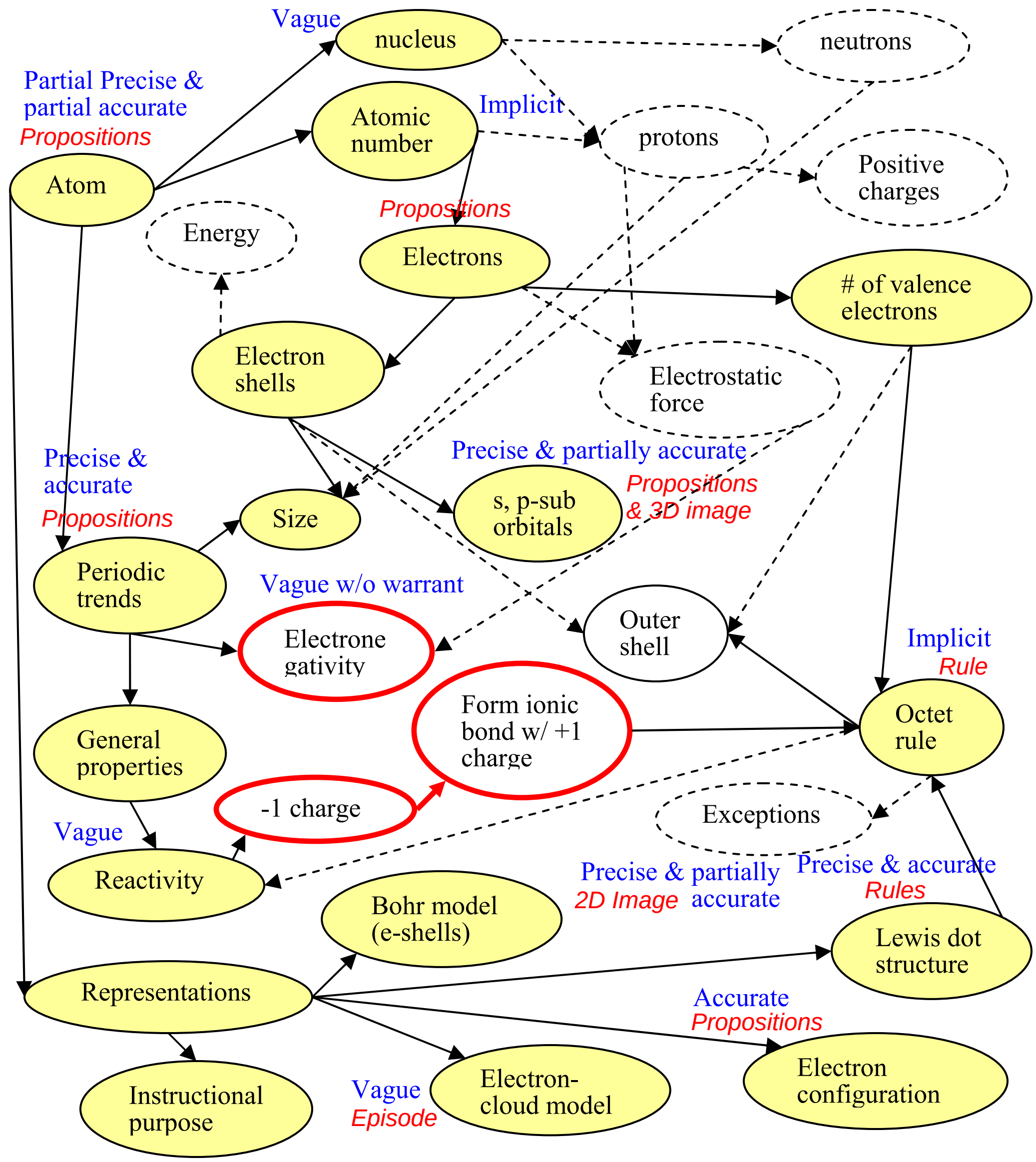


Figure 19. SD's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

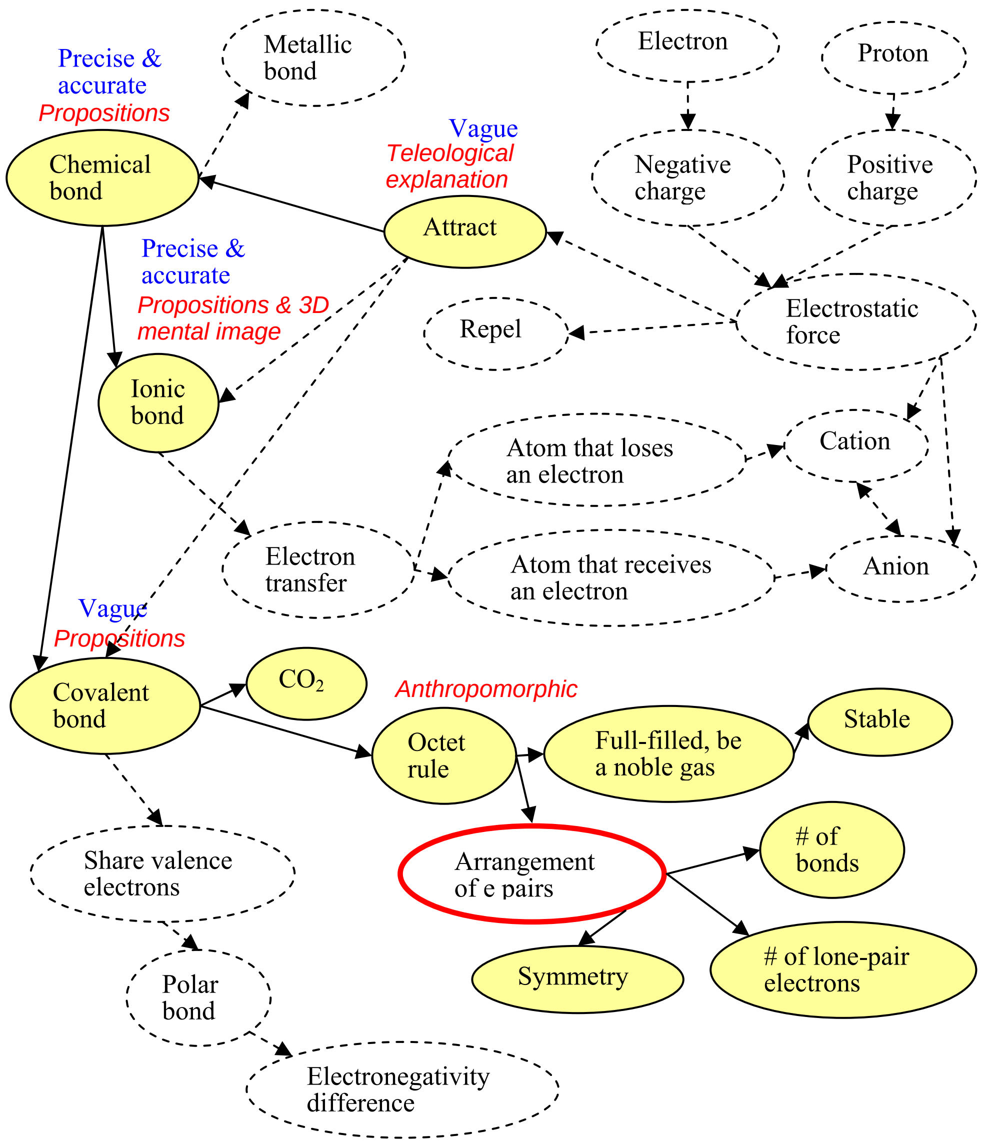


Figure 20. SD's concept web on chemical bonding.

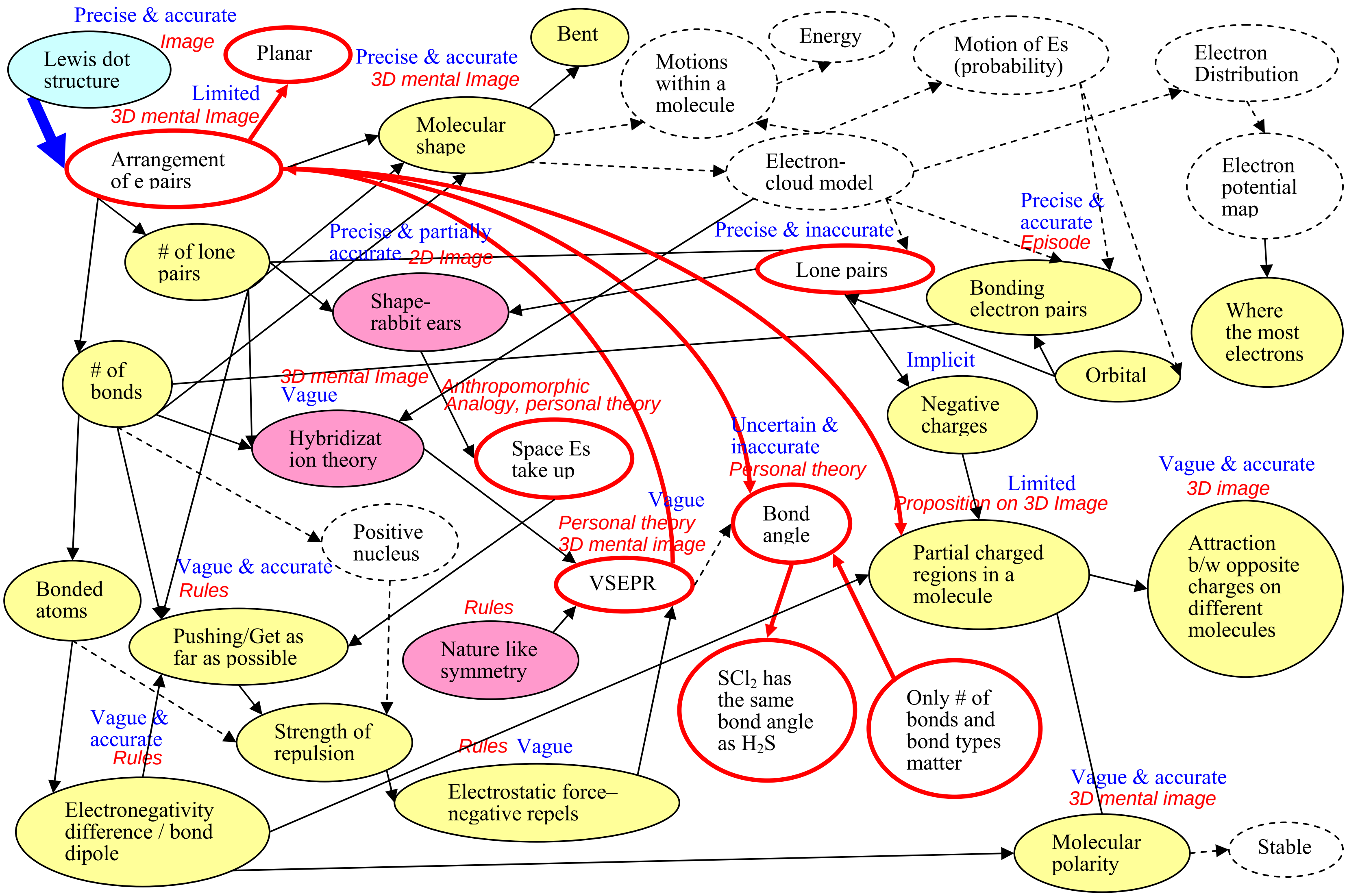
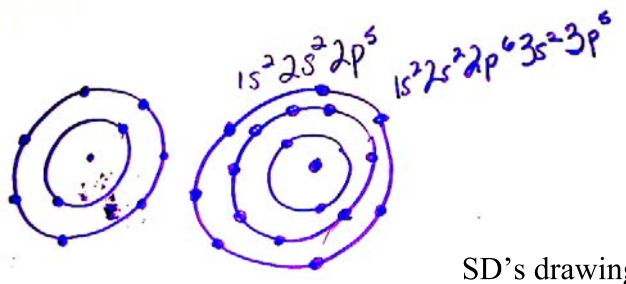


Figure 21. SD's concept web on molecular geometry and polarity.

Students in the moderate content knowledge group portrayed a Bohr model of a fluorine atom with the correct number of electrons on each shell, but used only a dot to represent the nucleus (Figure 22). When they moved on to describe a chlorine atom, they simply added another shell to the fluorine atom and completed the numbers of total valence electrons, disregarding the fact that the fluorine atom and the chlorine atom have different numbers of protons and neutrons.



SD's drawings

AM's drawing

Figure 22. Drawings of a fluorine atom and a chlorine atom for students in the moderate content knowledge group.

The missing role of the nucleus in an atom resulted from these students' deficiencies in understanding about interactions of electrostatic forces between the positive nucleus and negative electrons. The missing concept about the role of a positive nucleus in SD's conceptual framework was evident by her responses to instrument EN (EN-5, 10, & 11). SD and AM shared the following misconceptions about interactions of electrostatic forces: Neither associated an inner electron shell with a lower energy level (EN-2 & 9) or less electron-shielding effect (EN-7), nor understood an inherent property of Coulombic principles between the nucleus-electrons interaction--when a force acts between two bodies, both bodies experience the same magnitude of force (EN-6, 8, 13, 14, & 16). SD and AM also possessed an alternative conception about "conservation of force" (Taber, 2003) thinking once an electron was removed from the electron shell, a certain amount of attractive force would be shared among the remaining electrons (EN 15, 17, & 19).

SD's and AM's examples provide strong evidence that understanding the role of the positive nucleus is crucial when learning concepts about atomic structure. It is a bridging concept to understand concepts related to principles of electrostatic force and energy when a student develops his or her conceptual frameworks.

Their insufficient understanding about the atomic structure disadvantaged these students' comprehension about periodic trends. Unlike their peers who were able to connect their understanding about atomic structure to concepts of periodic trends, SD and AM were aware that elements in the same group shared similar chemical properties, but they could not specify the details. Periodic trends of reactivity, atomic radius, and ionization energy were missing from the descriptions of the moderate content knowledge students. For example, when AM was asked to describe similarities and differences between a fluorine atom and a chlorine atom, she could not give more specific descriptions than "chlorine and fluorine are in the same column… and their weight are different" (AM, interview), and she continued:

> I do not know much about the differences and similarities between the different, like in the columns and stuff. I do not know much about those. But the only, the only similarities is that they are in the same column, the same chemical properties, and they act the same. When like combine with other groups and columns. (AM, interview)

SD experienced the same difficulty while indicating the relative strength of electronegativity for the fluorine atom and the chlorine atom. The following conversation illustrates how SD's insufficient understanding about atomic structure disadvantaged her from conceptualizing the concept of electronegativity:

> SD: Their electronegativity is going to be different because they just in different spots in the chart [the Periodic Table]. And chlorine…which one is more electronegative? But like the highest one I think is chlorine, that's the highest electronegative.
>
> I: Why is it higher electronegativity?
>
> SD: Um…let's see if I remember. Like, he tried to explain it and then I got confused...Maybe it is more electronegative because of its size.
>
> I: The size of the nucleus or the size of the electron cloud?
>
> SD: I think it has something to do with size, but I'm not sure which, like as far as, I think it is electron cloud like, that has a lot to do with it. But…that's what I get, kind of reaching my edge of knowledge. (SD, interview)

In general, AM could compare the relative strength of elecctronegativity for sulfur, hydrogen, and chlorine based on their positions on the Periodic Table. Due to the fact that the role of positive core charge was missing from the moderate content knowledge students' conceptual frameworks, these students conceptualized the periodic trends as rules of thumb. The links between properties of elements in the periodic trends and characteristics of each element's atomic structure were missing in these students' conceptual framework.

Although SD and AM both preferred the Bohr model when they explained atomic structure, they visualized an atom in 3D where electrons were moving in a cloud or circling non-stop around a nucleus. SD formed a hybrid model combining a Bohr model with an electron-cloud model. She said, "The Bohr model makes the electron cloud easier for me to understand...They [electrons] quiver and go off in their own little orbitals and make this big cloud" (SD, interview). Students with moderate content knowledge could not provide quantum mechanics descriptions, and were unable to reconcile the quantum mechanics descriptions with the electron-cloud model. Due to a lack of confidence in their understanding about these two models, SD and AM preferred a model that they were most familiar with, the Bohr model, to reconcile new information or to solve a problem. The following two quotes at two different points during the interview explained why SD preferred a Bohr model:

> In my mind, when you say fluorine, that's [the Bohr model] what shows up in my head. Every time like that is what is going to pop up, because that's the first thing I learned. In my junior chemistry class in high school, this was the first thing I learned so…Well this is how you figure out certain things, this is what I learned first. (SD, interview)
>
> Like I understand these [electrons] aren't like…, they're not just perfectly arranged [in a Bohr model], they're in their little clouds and they move and stuff. But I mean, that's [a Bohr model] easiest for me to see it as far as, okay this one [chlorine atom] is going to be bigger, has more electrons because of how it is set up [in a Bohr model]. (SD, interview)

Chemical bonding and the octet rule (refer to AM's and SD's concept webs of chemical bonding). The deficient understanding about interactions between the positive nucleus and negative electrons hindered moderate content knowledge students' understanding about chemical bonding. SD and AM could not justify chemical bonding with the electrostatic force. Instead, they provided vague descriptions referring to a chemical bond as "two atom things that are put together by some attractive force to one another" (SD, interview), or "they share or transfer electrons and stuff" (AM, interview). When SD was probed further, "Where does force exert to keep the atom of carbon and oxygen together in the CO_2?", she answered:

> It is because the oxygen wants to be bonded, so they can be happy and the carbon wants to bond so it can be happy. So then they form bonds with each other, whatever means necessary to form a little bond. [8:04-8:47] (SD, interview)

The missing concept about electrostatic force left a void in the moderate students' conceptual framework. Therefore, the prerequisite concepts, such as interactions between positive nucleus and negative electrons were not available to support students' comprehension about chemical bonding.

A low quality of understanding about chemical bonding was evident in several places in AM's and SD's responses to instrument CB. Both students had difficulties in differentiating covalent bonding from ionic bonding (CB-5ab, 6ab; a and b indicated the content part and the reason part of a two-tier item, respectively). They shared the same misconception that "electrons are shared equally between two atoms in a polar covalent bond" (CB-1ab, 7b) without considering electronegativity difference between the two bonded atoms. Also, examples of chemical bonds given by these students were limited to covalent bonds such as O_2, Cl_2, or CO_2.

AM's responses to the interview questions and items on Instrument CB revealed that conflicting ideas about bond polarity existed in her conceptual framework. During the interview, AM associated the bond polarity of B-F bonds with the electronegativity differences between the boron atom and the fluorine atoms.

However, her responses to some items in Instrument CB showed contradicting results, such as "electron pairs must be shared equally in the H-F bond" (CB-1b), and the polarity of the oxygen-fluorine bond is best shown as δ^- O—F δ^+ because "oxygen has six outer shell electrons and fluorine has seven outer shell electrons" (CB-2ab).

While constructing a Lewis structure for a given molecule, SD and AM viewed the octet rule as a rule to follow. They justified it with a teleological reasoning (Talanquer, in press) thinking "every element wants a full octet, so they want eight electrons to be stable. Because the noble gases are the most stable, and they have eight electrons" (AM, interview). One difference between students in the high and moderate content knowledge groups was that students in the latter group were somewhat uncomfortable and showed a lack of confidence when dealing with an octet rule exception–a BF_3 molecule. For example, after SD drew a Lewis structure for BF_3, she looked at her drawing for few seconds. She then said:

> For some reason I want to put an electron pair here, but I do not think it is right because it [boron] only has three valence…They'd bond here but then that does not fill up the octet rule. So I gotta figure out what I'm doing here. Because…I mean it should fill, you should have eight on this one [boron atom]. And you have eight here, you have eight here [a fluorine atom], you have eight here. So I mean…I guess that works, I mean and that one isn't….fulfilling its octet rule. Wow, that's weird. [20:14-22:48] (SD, interview)

It was apparent that SD attempted to generalize the octet rule to the BF_3 molecule, but she realized that the conditions of the boron atom did not support the octet rule. This overgeneralization about the octet rule may result from these students' unfamiliarity with criteria and restrictions for applying the octet rule. Consider SD's explanations:

> There are some exceptions [about the octet rule]. But all in all, you usually want to form double bonds, triple bonds, to try and get it to do the octet because that's ultimately what they want to do anyways. They want to get to the most stable that they can get, which is…having eight in their valence…it would be a noble gas. [20:14-22:06] (SD, interview)

Throughout their interviews, there was no place that AM and SD specified the guidelines for application of the octet rule or cases of possible octet rule exceptions.

Molecular shape and molecular polarity (refer to AM's, and SD's concept webs of molecular shape and polarity). Students with moderate content knowledge indicated a notion of repulsion between electron pairs when thinking about the arrangement of electron pairs for a given molecule. They were also aware that the lone pairs generated greater repulsion than bonding pairs. Due to their low quality of understanding about principles of electrostatic force, these students could only partially conceptualize the VSEPR model with the principles. Therefore, AM and SD each developed a personal version of the VSEPR model, and these personal notions of the VSEPR model interfered with their determination of geometric structure for the arrangement of electron pairs (*Step 1*). Once the students had determined the molecular geometry, they applied a proposition of "pulls of electrons" and followed similar procedures as the high content knowledge students did to determine the directions and strength of pulls. Then they canceled these "pulls" spatially to determine polarity of the molecule (*Step 2*).

In the following subsections, I describe how AM's and SD's personal version of the VSEPR model influenced their thinking about molecular geometry (*Step 1*) as separated cases, and then discuss their mental models about bond polarity and molecular polarity (*Step 2*).

AM's Step 1. Differing from textbook explanations on the VSEPR model, AM believed that it was the atoms that bonded to the central atom. For example, the hydrogen atoms on a H_2S molecule repelled the lone pairs. When she explained the bent shape of a H_2S molecule, she said:

> The electrons [lone pairs] will repel the hydrogens…because it [lone pairs] is negative, so it...pushes away. So you put all electrons at top and it will be a bent structure…It [H_2S] would be like this [a linear shape] if there was no other charges on it, if it was like fully charged. But since there are two unbonded pairs of electrons, it does not attract these [hydrogen atoms], they repels them. So these [hydrogen atoms] were pushed down by the electrons [lone pairs], because they do not want to…they just get repelled. (AM, interview)

The above description led AM to believe that lone pairs and the hydrogen atoms were both negatively charged so they repelled each other. When she considered the electronegativity of the sulfur atom and the hydrogen atoms, she thought that hydrogen atoms would be partially positive because electrons were pulled toward the sulfur atom. The conflicting results about charges of hydrogen atoms confused AM in terms of whether the lone pairs would attract or repel the hydrogen atoms. To AM, either the VSEPR model or the electronegativity of each atom in the molecule could influence the molecular shape. This was evident by AM's responses on instrument GP while determining molecular geometry. In one question, AM indicated that "the shape of the $COCl_2$ is dependent on the electronegativity of each atom" (GP-5). In another question, she thought that "the molecule SCl_2 is v-shape because repulsion between the non-bonding electron pairs determines the shape" (GP-3). AM could easily visualize the arrangement of electron pairs for H_2S as a tetrahedral shape. She recalled the bond angle as 109.5°.

> Because the electron geometry is tetrahedral, because it has four possible bondings for it. And I just memorize the chart that if it has four, it is 109.5. Because they are all going to repel, like the same. Like if I have actual four bonds on here, then they will all be equal. And since it is [lone pairs] repelling, so it [the bond angle] will be slightly less then 109.5 [21:30-22:41] (AM, interview)

SD's Step 1. SD formed a hybrid model for H_2S by combining a Lewis structure with hybridization of atomic orbital (Figure 23). She visualized each bond and lone pair as a tear-drop shape to represent a region of dispersion force and described this feature as "personal space bubble" (SD, interview). For SD, formation of a mental model had a purpose of illustration to help her to comprehend some propositional statements of the VSEPR model such as 1) "bonding and lone electron pairs repel each other" and 2) "lone pairs are stronger and they can push a little more than these little guys [the bonds with hydrogen atoms] can" (SD, interview). SD described the lone pairs:

I think of like how they'll have the little circle things that this space they take up. That's kind of like they're little own personal space bubble, and

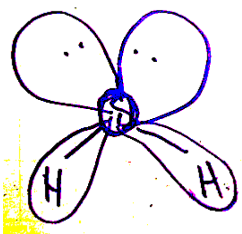


Figure 23. SD's drawing of a H_2S molecule.

> that helps me think of how that pushes this one [bond] closer to this one [bond]. [15:14-15:40] (SD, interview).

SD adopted the image of hybridization of atomic orbital to her mental model because "that was easy for my mind to see, so it stuck, so that's what I use, and I integrated it into other things" (SD, interview).

SD's mental model of H_2S contained incorrect spatial information by having the two lone pairs and two bonds on the same plane. Her planar mental model fulfilled the two propositional statements that she knew about the VSPER model. Therefore, she neither felt dissatisfied nor questioned the correctness of her planar model, even when I suggested the tetrahedral shape. She said:

> I do not know. In my mind, it is like this [planar]. But I mean it could, like if you rotated it around enough, it could essentially be kind of different looking. My little diagram, it is just always like this [planar]…because it is easier for me to see it that way. [3:45-4:49] (SD, interview)

SD's resistance on rejecting her planar mental model may be due to her misinterpretation about principles of electrostatic forces. Consider SD's explanations about her illustration of the lone pairs (Figure 24):

> I: Okay. So what's this within this little space (lone pairs)?
> SD: What's in the little space? Just them two [electrons], I guess. And then that's just my way of showing, they occupy this space, this is their space and this is….the forces that are repelling them from the other


Figure 24. SD's model of a H_2S molecule.

> thing. That's how much it goes and then, then it is okay, and after this point it is not going to push as much as they would otherwise. [18:31-18:52] (SD, interview)

When SD was probed further, she could not explain her drawing about "personal space bubble":

> I: But there are just two electrons.
> SD: Yeah, just two.
> I: How come it takes up so large space? So within this space where I can find those two electrons?
> SD: I…I did not think about it that far. I just…well…that's just how I got there, you know. It just… there's two of them [electrons] in there and that's how much space they take up in my mind and that's how it works. [18:31-19:24] (SD, interview)

SD adopted the representation of the hybridization of atomic orbital without understanding the quantum mechanics descriptions. Instead of conceptualizing the hybridization of atomic orbital as probability regions of electron distribution, she misinterpreted these bubble shapes as "boundaries of pushing." SD did not differentiate the concept of electrostatic potential region (the region that describes the degree of a charged object experiencing repulsion from another object with the same type of charges) from the concept of probability regions of electron distribution. This alternative concept about "personal space bubbles" hindered SD from applying the principles of electrostatic force to her mental model. Until her mental model is remediated to reflect a correct spatial arrangement and appropriate propositions, SD will not be able to use her mental model to engage in inferences about concepts of bond angle or molecular polarity. Evidence had shown that SD had difficulty conceptualizing the bond angle of H_2S. She tried to recall from her memory that the bond angle of a bent molecule was 120°. I then challenged her planar mental model for H_2S by asking "Since you have two lone pairs [and two bonds on the same planar], it [the bond angle] is supposed to be 90 degree. How come it is not?" SD said:

> Because they [two bonds] start out at like 180° and then you get those two [lone pairs] in there and they push down. And they do not push it down so much that it is like…90 degree to me. I may be wrong though because I may just be remembering wrong. I do not know why it did not push into it. [3:06-3:42] (SD, interview)

SD applied the proposition that the two lone pairs repelled the two bonds, but she did not realize the missing connection between a) effects of repulsions among the electron pairs and b) the structure of the molecule in 3D. SD, again, experienced the same difficulty when thinking about whether the geometry of BF_3 should be a right trigonal planar or a T-shape arrangement. Her responses to instrument GP indicated that she had difficulties constructing a correct Lewis structure and determining the arrangement of electron pairs for novel molecules such as NBr_3 (GP-1) or $COCl_2$ (GP-5).

Step 2. After using the VSEPR model to determine the geometry of a given molecule, AM and SD identified which atoms were more electronegative and which were less and determined the directions and strength of bond polarity (in their words, pulls of electron) for each bond. Students in the moderate content knowledge group visualized a 3D, uneven distribution of electron cloud with an electron-poor region around a less electronegative atom, and a electron-rich region around a more electronegative atom when describing concepts of bond polarity and molecular polarity.

For instance, AM adopted an electrostatic potential web to her mental model using colors from red to blue to represent the electron distribution from the electron-rich region to the electron-poor region. She indicated that a H_2S molecule was polar because:

> This [sulfur] is more electronegative, so it has partial charge up here. So here is a cloud around it. And this [sulfur atom] is a redder part and this [hydrogen atoms] is the blue part because it [sulfur] pulls more electrons toward it. It has a partial charge, positive up here. It has a partial charge and then it is polar. [20:20-20:44] (AM, interview)

Although AM mistakenly put a "δ^+" sign by the sulfur, she explained correctly that the sulfur atom "pulls more of the negative charges [electrons]" because the sulfur atom was more electronegative. She was able to distinguish that the sulfur atom did not gain an extra electron. "It is just more electronegative" (AM, interview). However, these students were not able to reconcile their mental model of electron-cloud with the quantum mechanism descriptions due to their lack of understanding about the latter model.

AM's mental-modeling ability allowed her to form a mental model as a thinking tool, to apply concepts to the model, and to adjust the 3D molecular shape accordingly. She was able to generate a mental model of BF_3 in a trigonal planar shape based on a T-shape, 2D Lewis structure and canceled out the directions and strength of bond polarity spatially. She explained:

> Boron is less electronegative. So it would pull that way [adding arrows from B to F on three B-F bonds in the 2D Lewis structure] But that's not...If I was looking at this structure [T-shape], I would say it is polar. BUT the bonds are actually all equal, equally space apart. So I will say it is non-polar because they're pulling equal amounts away. [25:55-26:40] (AM, interview)

In contrast, SD encountered a difficulty regarding visualizing a trigonal planar shape for the BF_3 molecule in 3D. The influence of this impediment to SD's understanding about molecular polarity demonstrated the interactions between an individual's mental-modeling ability and his or her content knowledge, and will be discussed in the section on interactions of mental-modeling ability and conceptual framework.

General descriptions about conceptual frameworks. Based on the analysis of concept webs and interviews, I found that students with moderate content knowledge had only a few misconceptions, but some key concepts were missing in the three conceptual frameworks such as influence of the positive core charges in an atomic model or principles of electrostatic force when describing chemical bonding. Their understanding about most of the concepts was accurate or partially accurate, yet were justified with vague explanations.

Sometimes these students followed rules of thumb (e.g., determining relative electronegativity of an atom using the Periodic Table) without justifying their approaches with appropriate propositions or with common sense explanations (e.g., teleological or anthropomorphic explanations). These students were somewhat satisfied with these partially accurate propositions, algorithmic strategies, and/or personal theories, rather than reconciling their incomplete understanding with textbook explanations. Thus some links between/among concepts were missing while explaining a concept or phenomenon, and their conceptual frameworks were semi-coherent and included some conflict concepts.

Students with moderate content knowledge possessed partial understanding about different models (e.g., Bohr model, electron-cloud model, and quantum mechanics descriptions), and were not able to describe in detail the meanings, explanatory power, or limitations of these models. This insufficient understanding disadvantaged students' reconciliations among these models. For the same reason, these models lost some degree of power for explanations or inferences, but still had power for illustrating propositions in these students' mind. Due to the incomplete understanding about models, students with moderate content knowledge preferred a simple model or one that they were familiar with while solving a problem. These students used the model "pop-up" in their mind when the given question triggered a specific model.

Conceptual Frameworks for Students with Low Content Knowledge (refer to TA's, KA's and JT's concept webs, Figure 25-33)

Among the eight interview participants, TA, KA, and JT possessed relatively less content knowledge about molecular geometry and polarity and prerequisite concepts. TA was originally categorized as a moderate-scoring student according to his scores on three diagnostic instruments. Analyses of TA's interview and his concept webs showed that several key concepts were missing from his conceptual framework. In addition, his explanations about molecular geometry and polarity were vague. He frequently used algorithmic approaches, and several explanations were erroneous or had no support. Therefore, TA was relocated to the low content knowledge group.

In this section, I describe concepts and the structure of conceptual frameworks of students in the low content knowledge group. Evidence from interviews of TA, KA, and JT and misconceptions identified from the diagnostic instruments are used to support my descriptions.

Atomic structure, periodic trends, and representations of atomic mode (refer to TA's, KA's and JT's concept webs of atomic model). Students with low content knowledge preferred symbolic representation while thinking about a fluorine atom. TA

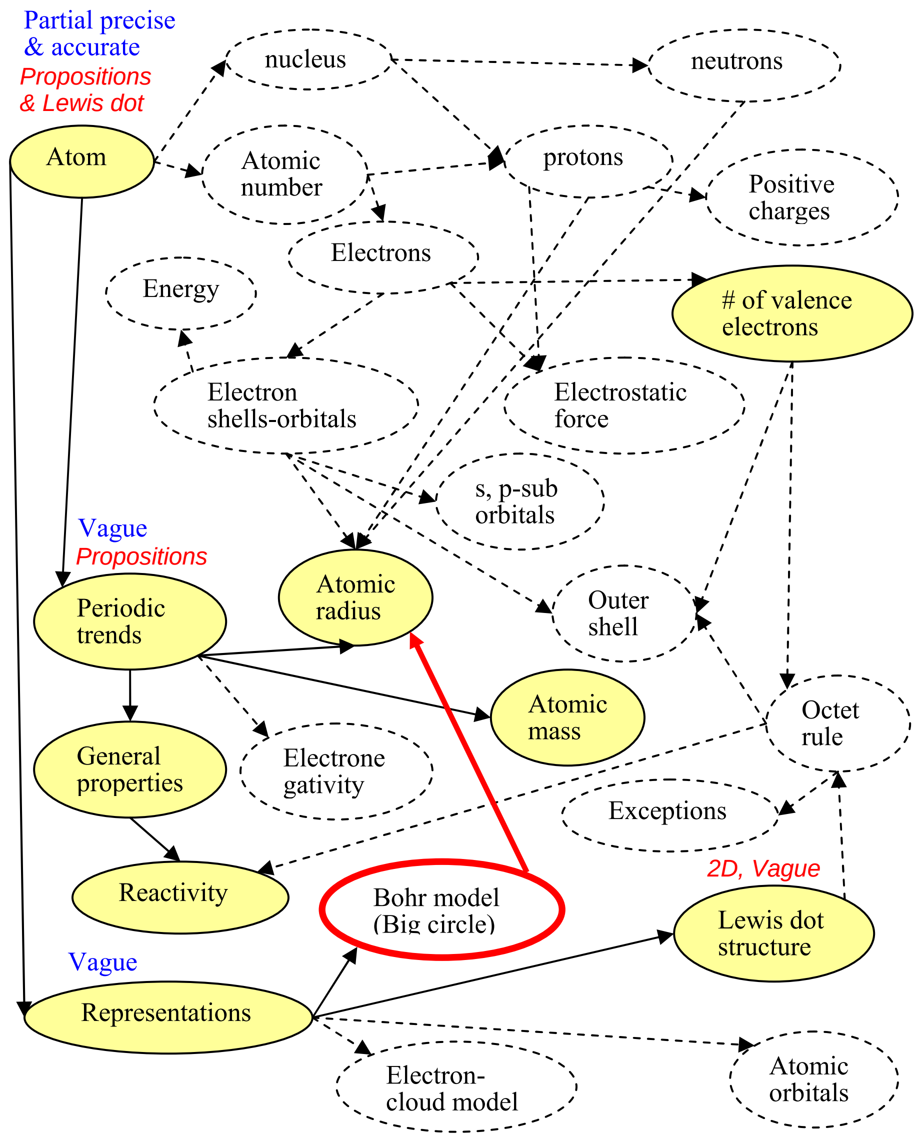


Figure 25. TA's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

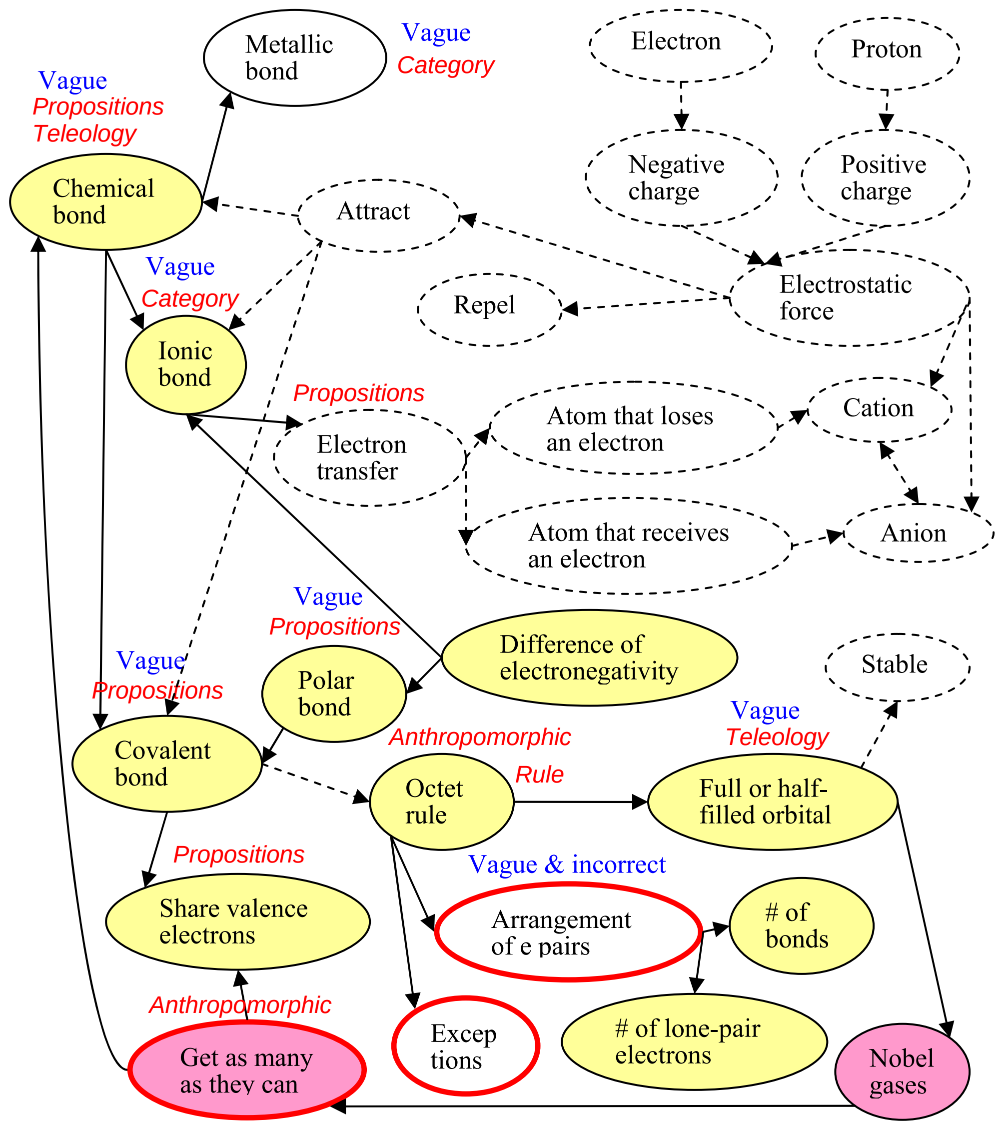


Figure 26. TA’s concept web on chemical bonding

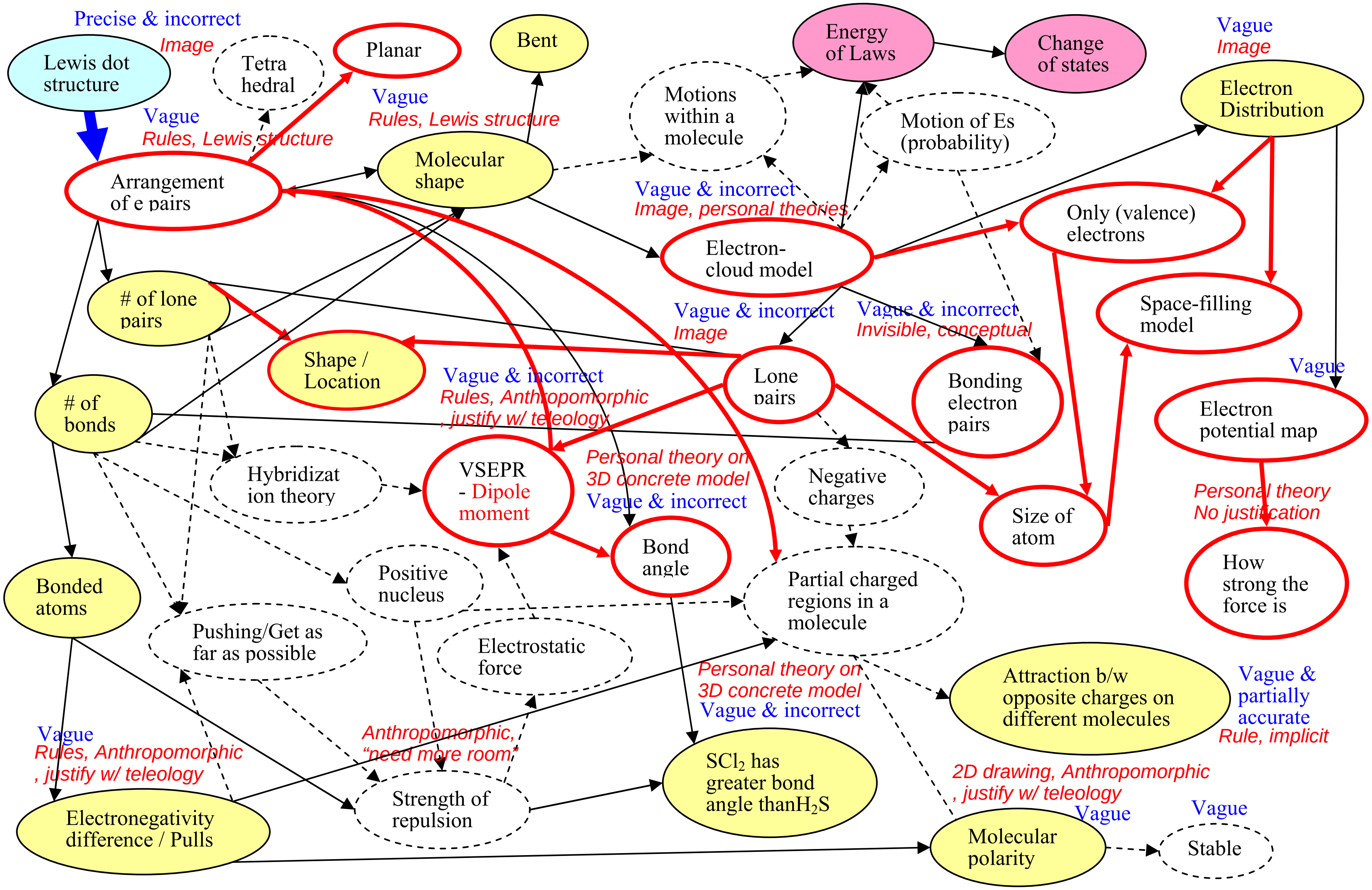


Figure 27. TA's concept web on molecular geometry and polarity

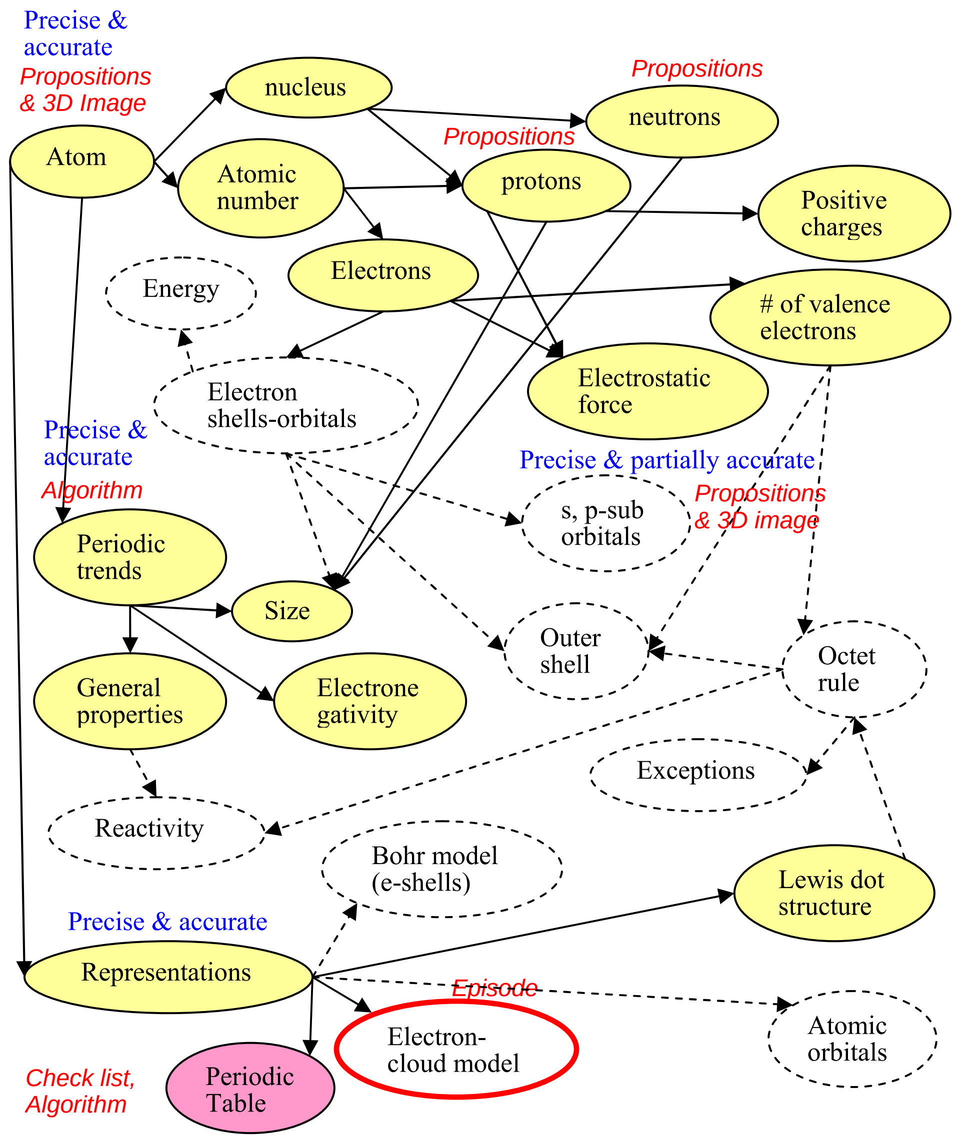


Figure 28. KA's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

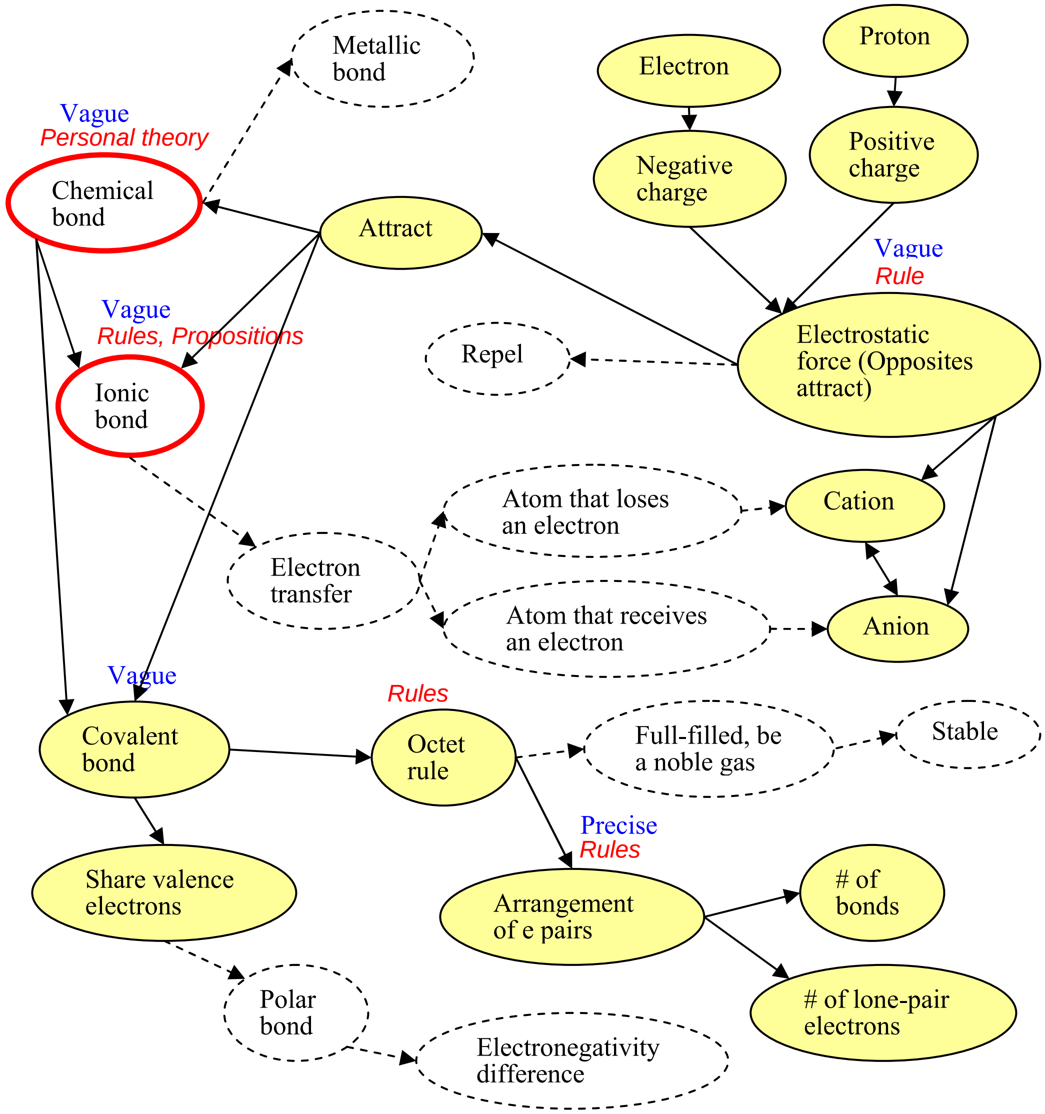


Figure 29. KA's concept web on chemical bonding

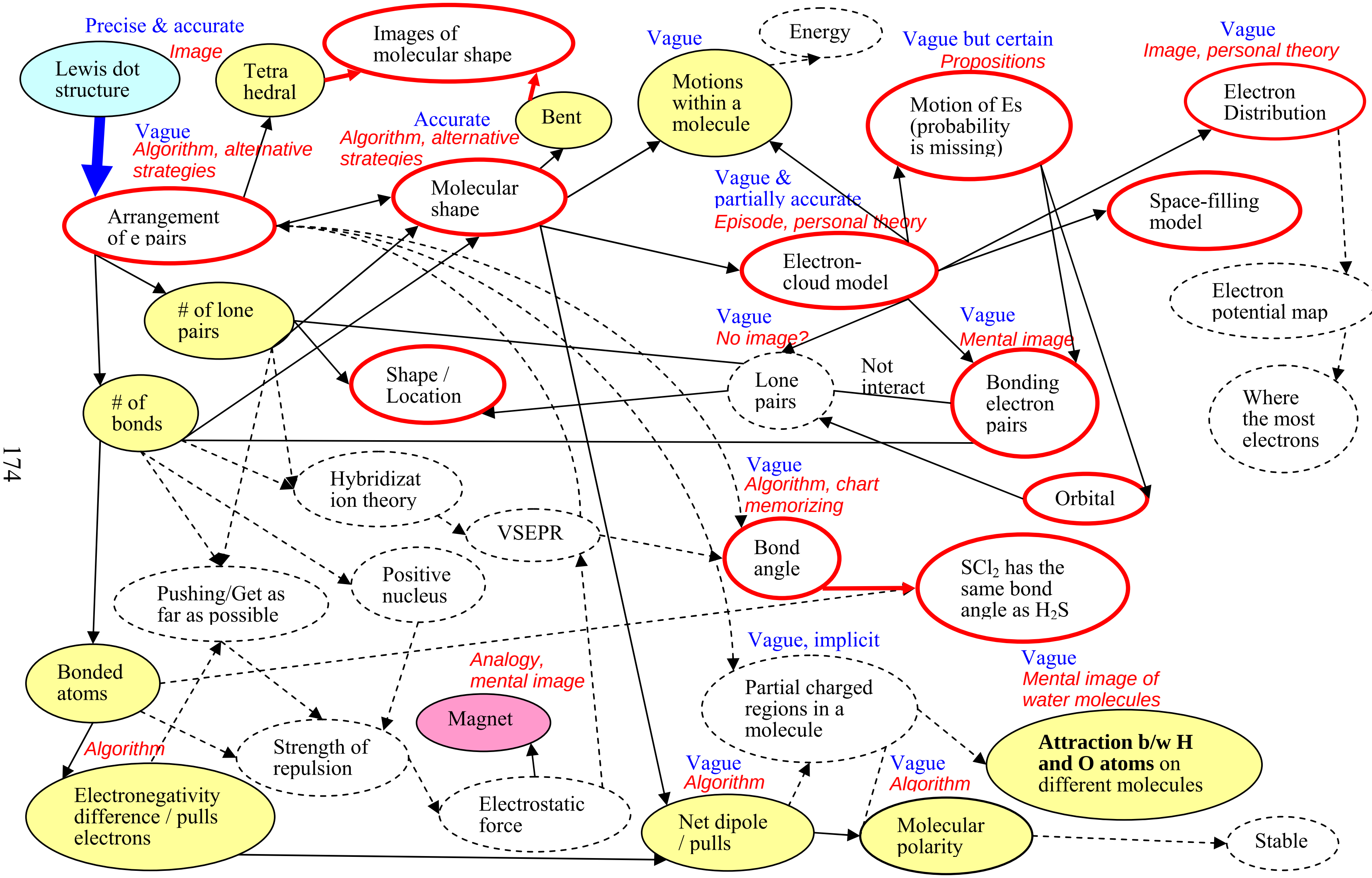


Figure 30. KA's concept web on molecular geometry and polarity

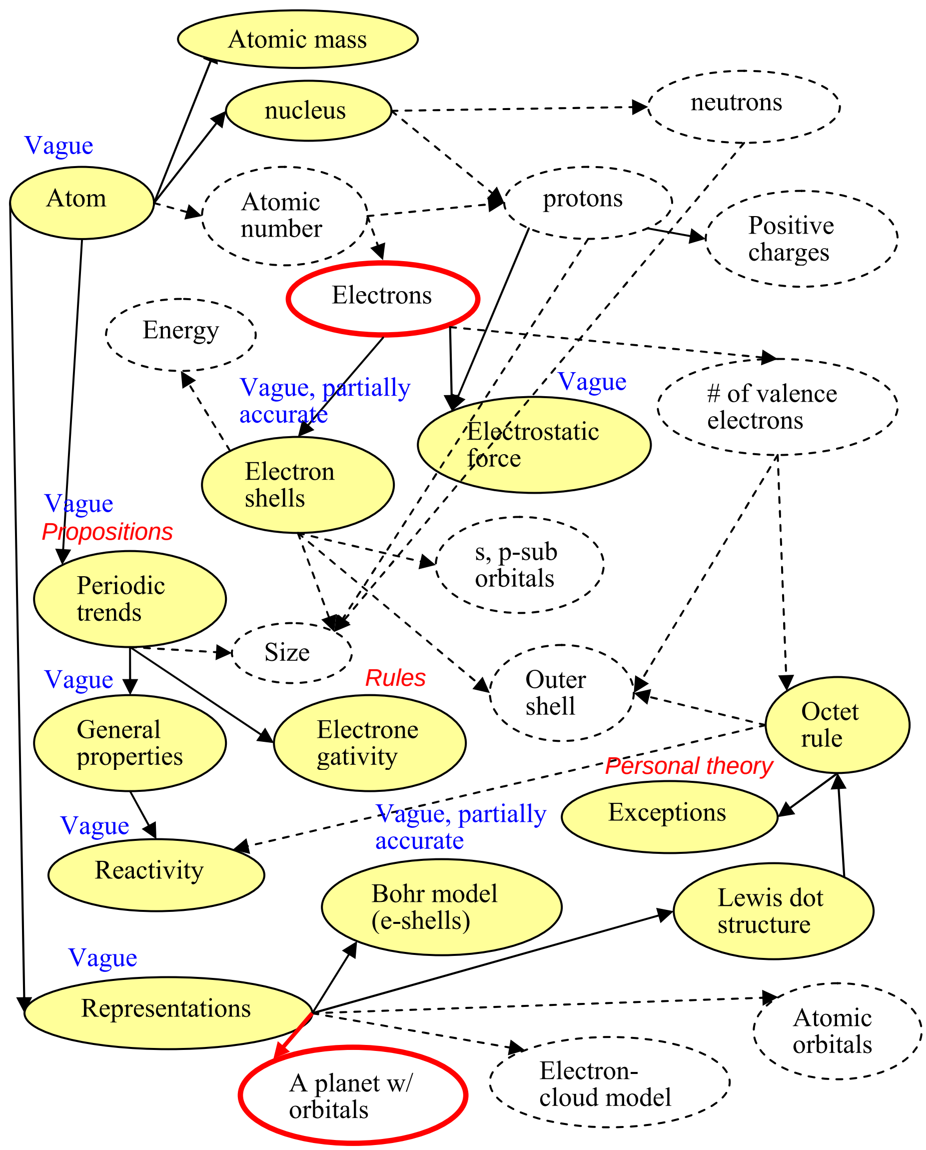


Figure 31. JT's concept web on atomic models. In the concept webs, ovals with solid line represent correct conceptions, ovals with broken line represent missing conceptions, and ovals with bold line represent misconceptions. Also, solid lines represent correct links, broken lines represent missing links, and bold lines represent wrong connections between concepts.

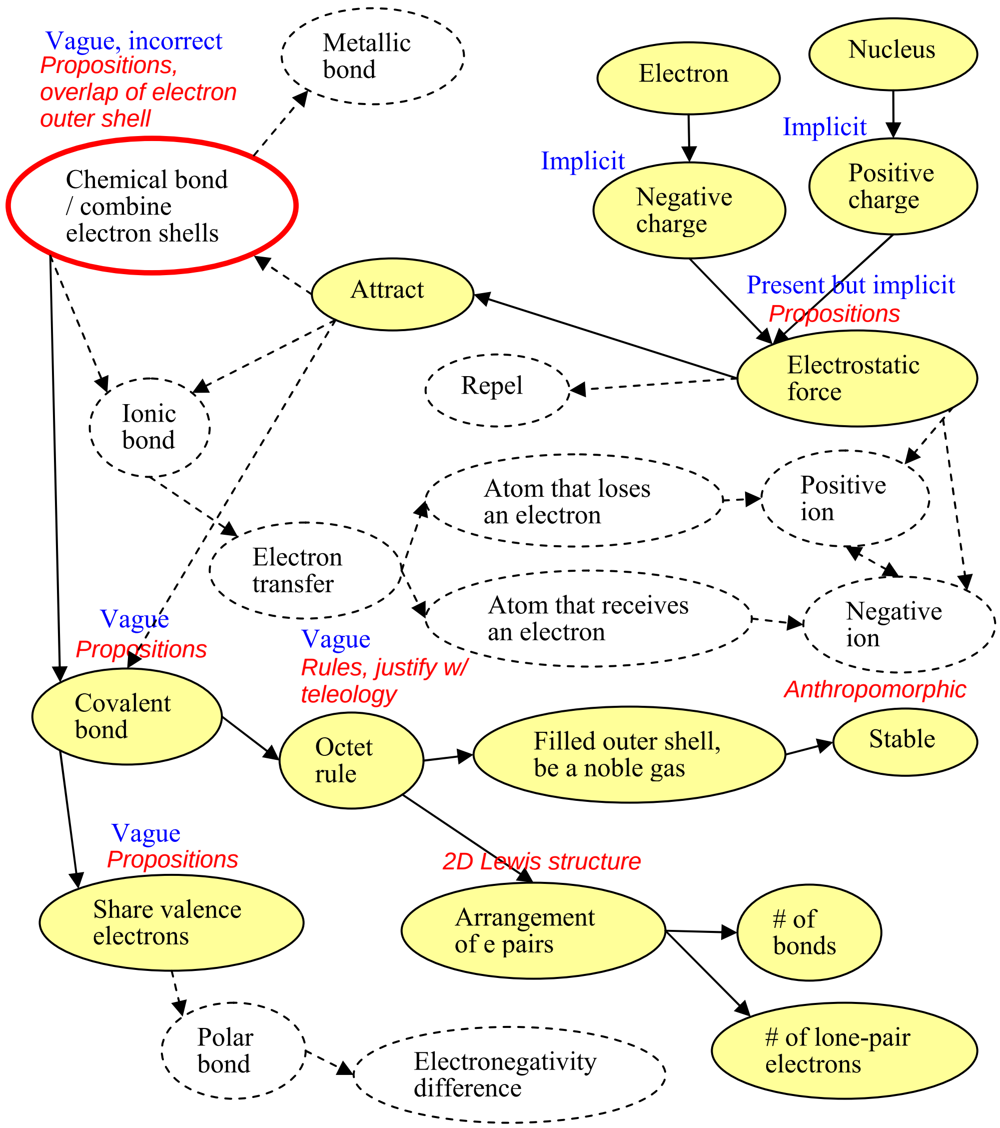


Figure 32. JT's concept web on chemical bonding

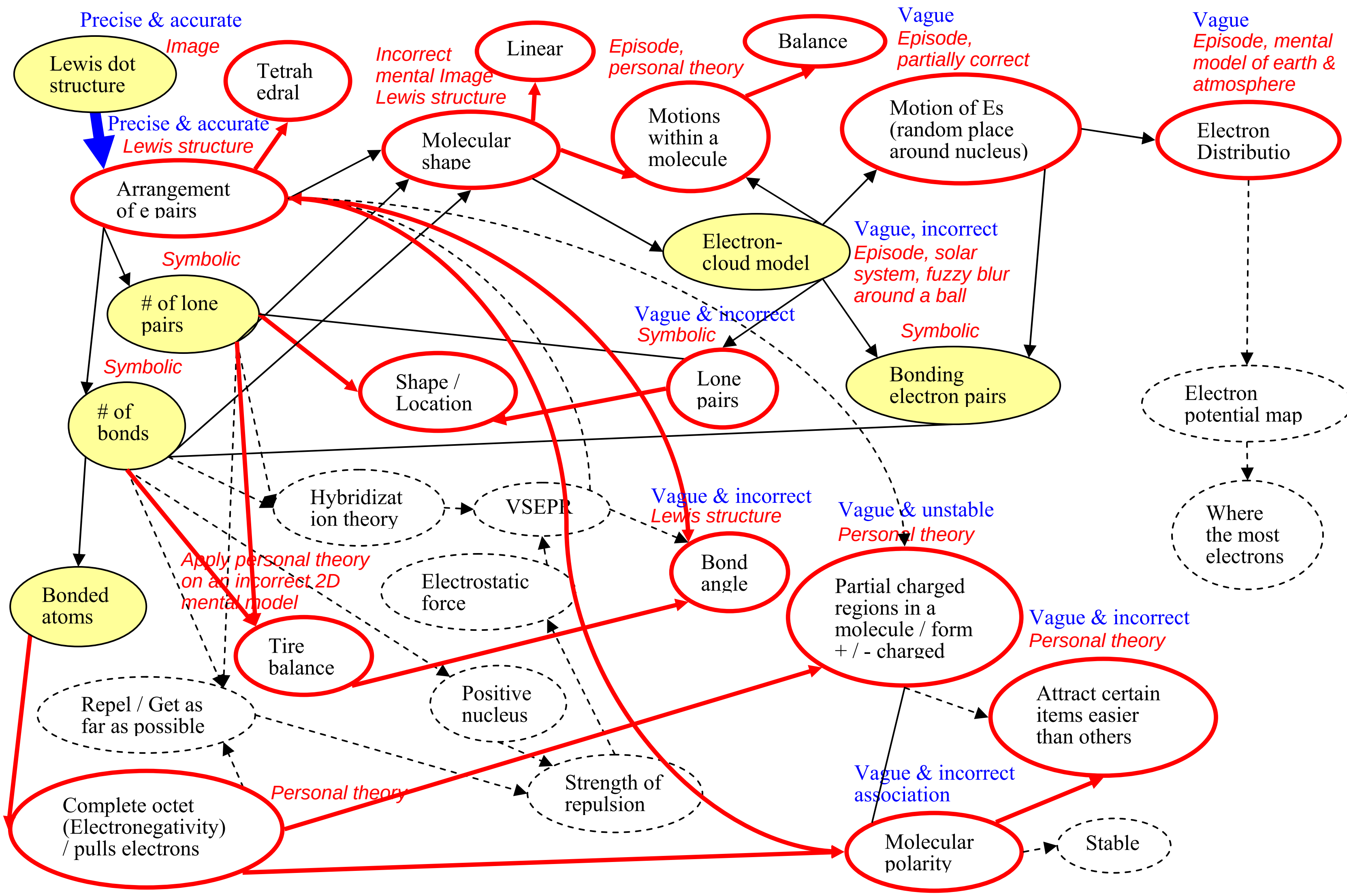
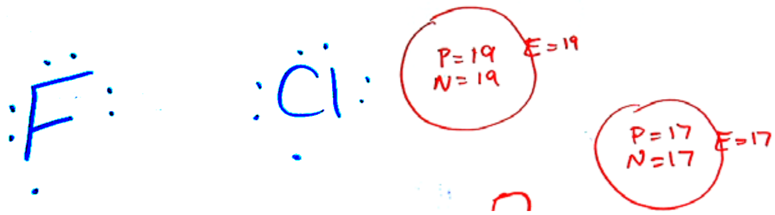


Figure 33. JT's concept web on molecular geometry and polarity



JT's drawings KA's drawings

Figure 34. Drawings of a fluorine atom and a chlorine atom for students (JT and KA) in the low content knowledge group.

and JT preferred simple Lewis dot structures, and KA used a special notion to indicate numbers of protons, neutrons, and total electrons (Figure 34). These symbolic representations did not reflect the appropriate structure of an atom, such as the Bohr model or a 3D electron-cloud model with a nucleus at the center and the electrons surrounding on the outside. The selection of representations also reflected these students' lack of understanding about concepts of atomic structure. Consider TA's descriptions about similarities and differences between a fluorine atom and a chlorine atom:

> The first things that come to my mind are just the Lewis structures. That's how I differentiate between different, you know…So like I do not really know how to differentiate between elements in the group besides just like a bigger circle basically, just because the atomic radius and so. [2:19] (TA, interview)

This deficient understanding was evident in their responses to items on instrument EN. TA, KA, and JT shared several misconceptions about interactions of electrostatic forces. They did not associate an inner electron shell with a lower energy level (EN-9) or less electron-shielding effect (EN-7). More or less they each responded to some items that indicated misconceptions about Coulombic principles for the nucleus-electrons interaction (EN-6, 8, 13, 14, & 16). Also, these three students possessed an alternative notion of "conservation of force," thinking once an electron was removed from the electron shell, a certain amount of attractive force would be shared among the remaining electrons (EN-15, 17, 19).

By using the Periodic Table, all three students were able to indicate the number of valence electrons and relative electronegativity for hydrogen, sulfur, boron, fluorine, and chlorine atoms. But due to their lack of understanding about atomic structure, these students could not conceptualize the periodic trends, such as reactivity, based on the characteristics of each element. For example, JT described that a fluorine atom and a chlorine atom "are in the same group so they have…I do not know exactly what but similar characteristics like they'd bond with other atoms in certain way" (JT, interview). Instead, these students memorized the trends in the Periodic Table algorithmically. KA's descriptions about his strategy gave a clear example:

> Just with the [imagined] Periodic Table being in front of me. Just from the stuff I learned from this year…I'm seeing arrows, like less electronegativity from left goes [right], from this [bottom], and this [to the top]; and the size goes from this and this; the radius, atomic radius. Just like first when from doing all these Lewis structure... I just go through like a check list, I guess. I do not think there's any image that's going through my head. It is just something memorized and applied. [3:30-4:07] (KA, interview)

When KA described the periodic trends, his finger was pointing in the air to draw arrows horizontally and vertically. Although KA raised a question to himself that "fluorine is smaller [than chlorine]; is it pulling the electrons closer to this nucleus?" he responded to instrument EN thinking that "the nucleus is not attracted to the electrons" (EN-5). KA possessed conflicting ideas that he knew that the electron was closer to the nucleus and would require more energy to remove (EN-2), and experienced less shielding from the nucleus (EN-7), but rejected the idea that the electron was in a lower energy level (EN-9). This evidence showed that knowledge existed in pieces in KA's conceptual framework.

Existence of fragmented conceptual frameworks was also observed in TA's and JT's cases based on their responses to instrument EN. JT understood that the electrons closer to the nucleus required more energy to remove (EN-2), but did not associate this idea with less shielding effect (EN-7) or the lower energy level (EN-9). TA was aware that electrons were attracted to a positive core (EN-5, 10, 11), but missed all the details regarding the nucleus-electrons interactions (EN-2, 6, 7, 9). KA, TA, and JT each possessed more or less misconceptions about the nucleus-electrons interactions (EN-6, 8, 13, 14, 16) and all shared the misconceptions on "conservation for force" (Taber, 2003).

Among the three students in the low content knowledge group, JT was an extreme case who had many concepts and links that were missing in his conceptual framework. His knowledge was fragmented, and details about propositions and models were lost from his memory. Thus, JT had memorized an atomic model based on its superficial features. For example, JT analogized the Bohr model to "like Saturn. I guess, like a planet. You have rings around it with the electrons on them" (JT, interview). He also saw the electron-cloud model "like Earth's atmosphere. If Earth is sulfur, and then I just picture a translucent enclosed sphere and around it where the electrons are going nuts, rotating around it pretty much" (JT, interview).

This strategy of thinking about atomic model using analogies was only for memorizing per se. Consider JT's perceptions about lone pair electrons when he reconciled a Lewis dot structure with an electron-cloud model:

> I'd say electrons are going every which way, so you could not really map that, which I think it is why they tell you to just stick them [lone pairs] on

> the side. I mean... They [lone pair electrons] are probably in random places around it [the nucleus] but it looks neater if you stick them next to each other. [15:46-16:17] (JT, interview)

Chemical bonding and the octet rule (refer to TA's, KA's, and JT's concept webs of chemical bonding). Students with low content knowledge described that chemical bonding as "a force that holds the elements together" (TA, interview); however, each of them held various ideas associated this concept. For instance, TA described a chemical bond as an "understood bond that they will form against each other. It is kind of like a magnetic force, and you can't really see" (TA, interview). Also, he applied a rule of thumb to calculate the electronegativity difference for a fluorine-oxygen bond and determined that it would be a polar bond because "there would be a .5 difference" (TA, interview). JT drew a Bohr model to conceptualize chemical bonding (Figure 35):

> Say that's the nucleus and just various shells. Just doing… how ever many shells there are…Like the closer in they [electrons] are, the stronger force pulling them in. So if you have electrons out here [on the outer ring] they're not pulling in towards the nucleus as strong as these [electrons on the inner ring] are because they're closer. So since these [electrons on the outer ring] are not as strongly pulled in, then they can bond with another one [atom]. And then since that one [halogen atom] only has one [electron] it needs to fill it, so it needs to pull on in from somewhere else at a stronger force. [5:54-6:07] (JT, interview)

Figure 35. JT's drawing of chemical bonding.

KA used word association to memorize the concept of chemical bonding thinking "covalent means to share electrons because the bond is made of two electrons," and visualized that chemical bonding was the overlap between electron clouds (Figure 36). When he described ionic bonding, he thought about:

> The charges. Like the cations and anions. Opposites attract, I guess in that way. The charges, they have to be balanced. So like hydrogen is +1 and fluorine is -1 so those match up. The charges would be the same and they like to be together. (KA, interview)

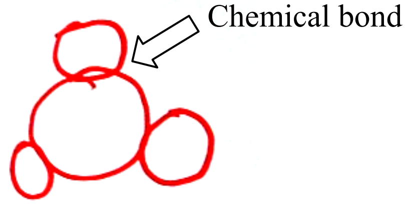


Figure 36. KA's drawing of chemical bonding.

This excerpt indicates that KA possessed a misconception about the electrostatic force thinking that the same amount of opposite charge would want to match up. He also gave a wrong example by discarding the fact that the bond between hydrogen and fluorine was a covalent bond rather than an ionic bond.

I felt that these low content knowledge students spoke whatever came to their mind at the time during the interview. Also, the concepts that they described were fragmented and inconsistent. These students neither connected their concepts in a meaningful manner, nor supported their explanations using appropriate propositions. Like KA said:

> I do not think I have ever thought of this so conceptually before. I just, I just seem to just to plug it on and try it, I never thought about it in much detail like this so I'm not too sure. [24:45-24:28] (KA, interview)

These students' responses to instrument CB indicated that they perceived sodium chloride, NaCl, as a molecule (CB-6a) and shared the same misconceptions with students with moderate content knowledge about "electrons are shared equally between two atoms in a polar covalent bond" (CB-1ab). In addition, TA, KA, and JT thought that the polarity of the bond was determined by the non-bonding electron pairs or the number of valence electrons on the bonded atoms discarding the electronegativity of the bonded atoms (CB-2b).

Similar to students in the moderate content knowledge group, these three students considered that the octet rule was a special rule to follow. Also, they provided teleological explanations about the octet rule to justify the formation of chemical bonds and a chemical compound. For example, TA described that atoms formed chemical bonds because "they want to get the eight full electrons, like the noble gases, so they want to combine to get as many electrons as they can" (TA, interview). JT used anthropomorphic terms to explain the octet rule that "the octet rule means eight. Since it has eight, it does not need an electron, and it does not need to lose one. It is happy, I guess. It is in its happy state" (JT, interview).

These students overgeneralized the octet rule and thought that "every element on the periodic table wants to try and be similar to the noble gases, which already have eight valence electrons" (TA, interview). Both KA and TA considered that the hydrogen atom as an exception of the octet rule because "hydrogen, never, does not have lone pairs" (KA, interview). Even though KA was aware of the nucleus-electron interactions when he talked about atomic models, he did not apply this concept to conceptualize the octet rule. TA's, KA's, and JT's responses to instrument CB revealed a strong commitment to the octet rule (CB-3, 4, 12, 18, & 20) which was consistent with their expressions during the interviews. To the students with low content knowledge, the octet rule became a rule to follow and exceptions of the octet rule were cases to memorize.

Molecular shape and molecular polarity (refer to TA's, KA's, and JT's concept webs of molecular shape and polarity). For students in the low content knowledge group, their procedures for determining geometry and polarity of a molecule included the following three steps: (1) use an algorithm to determine molecular geometry or think about the arrangement of electron pairs based on the 2D Lewis structure; (2) apply a proposition about electronegativity difference to the 3D or 2D molecular structure and determine the directions of “pulls” for each bond; and (3) cancel the “pulls” spatially and determine the molecular polarity.

Among the three students in this group, TA and KA employed similar algorithmic approaches, but they possessed different notions about molecular geometry and polarity. JT was an extreme case in that his conceptual framework was fragmented and included many misconceptions and missing concepts and links; therefore, he developed various personal theories during the processes of reasoning. It was hard to find common points between JT and KA or TA. Thus, in this subsection, I first discuss TA’s and KA’s cases on their determination of molecular shape and polarity. I then talk about JT’s case to demonstrate the thinking processes of a student without an appropriate conceptual framework.

TA’s and KA’s Step 1. TA and KA had poor understanding about the VSEPR model. For example, when TA explained the bent shape of the H_2S molecule, he said:

> Well, because of dipole moments. I mean that’s….we did not really go into depth on dipole moments. We just learned that whenever there’s a lone pair like this, like that [a bent, H_2S molecule]…That’d mean that there’s a dipole moment and those are pushing down. Because like if those lone pairs would not be there, then these would not need nothing else to have to go down, so they would just be a linear. But since there’s the electrons [lone pairs] up here, that they need the room, that they need the space because they have their outer shells, too. So that means that they will push down the hydrogens. [08:15-09:03] (TA, interview)

TA's explanation indicates that he possessed the notion that lone pairs repelled (pushed down) the hydrogen atoms. However, he could not use the principles of electrostatic force to explain this phenomenon, instead, he used anthropomorphic explanations such as "they need room, they need space". Also, TA did not understand the relationship between concepts of dipole moments and the molecular geometry; therefore, he mistakenly attributed the idea of dipole moment to the repulsions between electrons pairs that eventually determined the molecular shape. In KA's case, the analyses of his concept webs indicated that KA possessed partially accurate understanding about principles of electrostatic force. However, he neither applied the principles to comprehend the VSEPR model, nor associated the VSEPR model to the prediction of molecular geometry.

TA and KA had difficulties conceptualizing lone pairs as a feature of their mental or concrete model. They never illustrated the lone pairs when they constructed a mental model or concrete model of a H_2S molecule. When TA built a concrete model of a H_2S molecule, he described:

> Whenever you're doing these models, you do not show the lone [pairs]…so you would just, it'd basically look like that (Figure 37), and that would be its molecular geometry. And then you have to put in the perspective that there are two lone pairs. [07:15-07:57] (TA, interview)

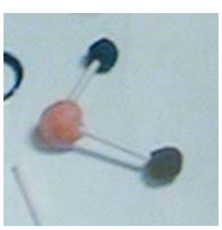


Figure 37. JT's model of a H_2S molecule.

To TA, the concept about lone pairs existed as a propositional statement such as "lone pairs were what's pushing the hydrogens down instead of keeping them in a line" (TA, interview), rather than a visualized image as a part of the features of a mental model. KA had the same impediment while visualizing the lone pairs on the H_2S molecule:

KA: Oh. There will be electrons [lone pairs] there, I guess. I know there are electrons there. I just do not see it when you draw the bond stick model.
I: Tell me more. I'm not sure I get what you're saying.
KA: I do not know how to explain it. I mean there are electrons [lone pairs] there but I would not know how to go into detail why you do not see it there or is it there.
I: Okay. Since you told me these are the lone pair electrons. Where are the lone pair electrons in this model?
KA: They're still on there, like…I mean they're still there.
I: Where? Which part of this molecule can I find these [lone pairs]?
KA: It would be on the sulfur...It would still be around. Like, electrons would still belong to the sulfur, and it would be like floating around or whatever…I think they're just floating free but still within that gravitational pool or whatever it is called. [21-51-23:36] (KA, interview)

The above conversation shows that KA neither saw the geometry of arrangement of electron pairs as a tetrahedral shape, nor visualized the two lone pairs as two probability regions of electron distribution. Although he knew from the Lewis structure that H_2S consisted of two bonding pairs and two lone pairs, the missing concept about quantum mechanics description of electron distribution hindered his visualization and comprehension about the hybridization of atomic orbitals.

Quantum mechanics description is a critical concept to understand the concept of a probability region of electron distribution. And the concept of a probability region of electron distribution is fundamental to comprehend the hybridization of atomic orbital and the VSEPR model. TA and KA did not have these prerequisite concepts to support their reconciliation between the Lewis structure and the 3D geometry of H_2S based on the VSEPR model. Thus, the questions about “Why there were four bonding sites on the sulfur atom?" and "Why the two lone pairs were considered as two regions of electron distributions that repelled the two bonding pairs in a tetrahedral geometry?" were mysteries to them. Consider KA's descriptions about lone pairs on the H_2S:

> I think maybe the two lone pairs do not interact at all between the bonds. I think where the bond site is at that the lone pairs would never interact with that site [H-S bond] or whatever. So they [lone pairs] are still there, but I said it [electrons] is moving, I mean it is nature, it is not going to cross that site or whatever. [28:31-28:53] (KA, interview)

When the gap of reasoning between the 2D Lewis structure and the VSEPR model was too big to fill, these students started to operate their thinking based on intuitive reasoning. For example, TA was aware that there were repulsions among lone pairs and bonding pairs, but he did not bridge this concept with the VSEPR model. When he was prompted to consider whether the arrangement of electron pairs for H_2S should be planar or tetrahedral, he said:

> Actually, it would be like that [tetrahedral]. Because it…I just have a feeling that it would be like this [tetrahedral] but I do not know why. I can't think of why it would be like that. But I just have a, I have a really strong feeling that it would be….yeah. [26:02-26:38] (TA, interview)

When TA compared bond angle of SCl_2 to the bond angle of H_2S, he was able to apply the notion of repulsions existing among bonding pairs to the mental model, and predicted the bond angle of SCl_2:

> They would change…Well they would, the angle would become bigger because they [Cls] would spread out more, because these [lone pairs] are the same size. So then instead of them [lone pairs] being up here pushing down, they [lone pairs] would give them [chlorine atoms] more room because they [lone pairs] would be the same. So they [all electron pairs] would all even out and be 90 degrees, well unless it would be like this [tetrahedral]…because then those would all be 109…No, they'd be 120… yeah, those would all be 120 angle. [26:49-27:58] (TA, interview)

Despite the fact that he used the anthropomorphic terms such as the lone pairs would "give them more room" to imply that chlorine atoms had stronger repulsion than if there were hydrogen atoms, TA demonstrated the ability to impose a proposition to the model and manipulate the model accordingly. However, he still possessed the inaccurate mental model that the four electron pairs would even out on a 2D plane. TA neither was ready to reconcile the spatial information of the tetrahedral geometry to his mental model, nor to comprehend the bond angles of the tetrahedral shape mathematically. Thus he continued to rely on rote memorization to recall the bond angle as 120°. The low quality of TA's conceptual framework failed to support him in terms of making the final decision between the planar and tetrahedral geometries.

KA, who used an algorithmic strategy most of the time, again used an algorithm to recall the corresponding bond angles for a H_2S molecule with a tetrahedral geometry in his mind, yet could not remember the details. He described his thinking process: "I thought of...I just went through linear is 180 [degree], triangle is 90 [degree], and that's where it stops. I could not think of…I just stopped there. I could not think of what it was" (KA, interview). When KA had an opportunity to access the textbook, he found the information quickly and indicated that the bond angle of a H_2S molecule was 109°. KA failed to consider that lone pairs in the H_2S molecule had greater repulsion than bonding pairs. When he compared the bond angle of a SCl_2 molecule to that of the H_2S molecule, again KA went through the algorithmic strategy:

> KA: That's how the molecule [SCl_2] would look like. It'd still be, ya, tetrahedral and it'd still be bent.
> I: Did you still go through the two/two strategy [algorithm]?
> KA: Umhunn.
> I: Okay. Since this molecule will still be bent, would the bond angle change? Would the bond angle be different from that one [H_2S]?

KA: No.
I: But you said the chlorine is bigger and the hydrogen is smaller, would it make a difference to the bond angle?
KA: I would not think so. I would not think so. No. [4:34-4:42] (KA, interview)

It was evident that this habit of algorithmic reasoning hindered KA from considering the additional conditions added to the problem (in this case, the relative size of chlorine atoms compared with the hydrogen atoms). Prior experiences with success in using an algorithmic strategy to solve problems had established truths about outcomes of this strategy in KA's mind.

TA's and KA's Step 2. TA and KA identified the relative electronegativity of atoms in the given molecule using the Periodic Table and determined the directions of bond polarity. However, they simply followed an algorithm that "whichever one's more electronegative is what will pull greater" (TA, interview), without conceptualizing this property of electronegativity with the positive core charge of an atom. As LMMA students, TA and KA drew arrows along the bonds on paper pointing from less electronegative to the more electronegative atoms instead of generating a mental model while thinking about bond polarity (refer to the section on LMMA students on p. 124).

KA thought of a polar molecule that "there is a direction where the molecule is being pulled more at...I just think of a pull like its pulling away, maybe" (KA, interview). Similarly, TA conceptualized a polar molecule as a molecule that had a sum of uneven forces resulting from its unsymmetrical geometry. To explain the concept of the polar molecule, TA gave a counter example, a CCl_4 molecule, and used an analogy about tractors pulling to explain the idea of balancing forces. He said:

> If you have the fluorine and carbon…that would be a non-polar because… Since all of these [chlorine atoms] are equal in their electronegativity,

> they're all going to pull their own ways, and there won't be any…like, the way that my professor taught me was like with a tractor. Like if say these are all like tractors or trucks or something pulling, that they all have the same force, so there's nowhere that any of them can go because the way they're set up. So that would be an example of a non-polar. And that [H_2S] would be an example of a polar because of the way of their molecular geometry…that they're pulling downwards so it would slightly pull the sulfur downward. [13:53-14:53] (TA, interview)

With this tractors-pulling analogy, TA conceptualized the notion of zero dipole moment for a nonpolar molecule as "there's nowhere that any of them can go."

In this paragraph, I only report TA's responses because KA did not participate in instrument GP. TA's responses to items in the instrument GP indicated that his thinking processes about molecular geometry and polarity were inconsistent. Sometimes, TA took the geometry of H_2S into consideration when determining its polarity during the interview. Other times, he correctly indicated that ClF_3 and OF_2 were polar molecules (GP-6a and GP-2a, respectively), but attributed the reason to the high electronegativity of the fluorine atoms (GP-6b and GP-2b), without considering the influence of geometry. Moreover, in contrast to his responses to GP-2a, TA thought that the strength of the intermolecular forces was greater between CF_4 molecules than between OF_2 molecules because there are four polar bonds in CF_4 and only two in OF_2 (GP-8ab). This suggested that either TA responded to instrument GP thoughtlessly, or he was operating on a fragmented conceptual framework rather than a consistent, logical thinking process.

JT's case. JT was an extreme case that represented a student who did not have appropriate knowledge to conceptualize problems about molecular geometry and polarity. He neither understood the VSEPR model nor visualized 3D geometries other than his drawings of 2D Lewis structure. JS determined the geometry of a given molecule based

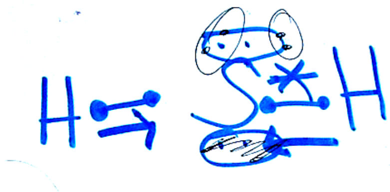


Figure 38. JT's drawing of a H_2S molecule.

on its 2D Lewis structure. He identified which atoms were more electronegative and which were less and then determined directions and summed up the "pulls" to see if there was force remaining to stretch or bend the molecular shape. The following conversation demonstrated how JT decided that the H_2S molecule had a linear shape:

> I think that [H_2S] would be a linear [Figure 38] because like these [bonds]…it is pulling in [from H to S]. Since it is equal on both sides, it
>
> cancels each other out, because they're pulling in at each other at the same time. So that cancels. Since there is a lone pair on each side…So one lone pair and two lone pairs and those cancel each other out. That means there is no force stretching it or bending it. That's linear which means its angle is 180˚. (JT, interview)

This approach for determining the molecular geometry was used by JT consistently throughout the interview and to solve related problems in instrument GP (GP-1ab, 3ab, 5b, 13ab, & 15ab).

JT formed a mental model to support the approach discussed above and this mental model was supported by an alternative conceptual framework. His model included a sulfur atom in the middle and two bonded hydrogen atoms on both sides with lone pair electrons floating and circling around the sulfur atom. JT further elaborated his mental model:

> One thing I've thought about is just like if you would think of balancing a tire on a car. If it is not balanced...you got this [he drew a circle, Figure 39] and say you just got electrons right there [on the circle] which would be a tire, a tire weight, basically. So as it rolls, it is not going to roll perfectly... its going to throw it off balance. And then if you add another weight on the

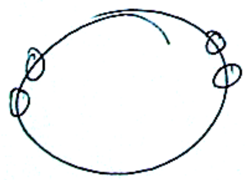


Figure 39. JT's drawing of a personal theory of tire-balancing.

> other side which is like another electron pair, then it will spin evenly because it won't... it won't throw its balance off. It will balance out this one that's throwing it off. I do not know if the atom will be rolling but that's what I think of. [27:46-28:53] (JT, interview)

JT had this vivid mental model that was tightly connected to propositions about tire-balancing and embedded in his alternative conceptual framework. Thus, it was hard for JT to give up his mental model. In addition, this mental model hindered him from accepting the bent shape of H_2S. Consider the following conversation when JT was reminded that the shape of H_2S was bent:

> I: If I told you that this molecule [H_2S] is bent, what may be the reason of that?
> JT: I'm trying to remember this from our lab because we did it. So that means it would get rid of this one [cross-out the lone pair below S], which I think we had this one [add another lone pair on top of S] and I messed it up. Since if the two electron pairs would be on top, it means it would basically look like that (refer to Figure 39).
> I: Have you thought about why these two lone pair would like to be on top?
> JT: No. I've wondered but I have no idea why. When I think of electrons rotating, again I can just see it as an equal…they're just always going around the S.
> I: Then it does not make sense that they [lone pairs] like to stay on top.
> JT: No. I have no idea. Unless there is polarity, I guess…Tying chemistry together! (JT, interview)

JT came up with an alternative explanation thinking that the two lone pairs and two bonds were all "polar." JT's wrong perception about lone pair electrons on a linear, 2D Lewis structure also led to erroneous inferences about bond angle. He said:

> I do not remember exactly what... but I wanted to say 120 [°]. That might be wrong. I think it is. Just because the way I look at it, I just think of a triangle. That's if there'd be two [lone pairs] up here then the 1, 2, 3, [lone pairs, one bond, and another bond] 360˚ divided by 3 is 120˚, which would be like 120˚ right there. I think it is wrong. I think that's wrong. I do not remember what it is but that is how I do the angles. [25:42-26:49] (JT, interview)

Later, when JT solved a problem about the shape of SCl_2, he soon gave up the idea about a bent molecule and fell back to his original mental model thinking that the shape of SCl_2 was linear.

JT's poor understanding also reflected on his idea about polar molecules. He thought that a polar molecule would "attract certain items more easily than others," and gave an irrelevant example about the cohesive force of water molecule:

> I think one example we learned, since water which is the same thing, which is why it is polar. Since they [water molecules] are similar, they stay close to each other but at the same time they push each other off just enough, which I think we learned in biology. That's why… I forgot the name of the bug, the insect…which is way it is allowed to walk on the water. Because of the polar characteristics of water. [8:19-9:20] (JT, interview)

JT represents a student who developed an alternative conceptual framework consisting of naïve theories and personal notions and models. This alternative conceptual framework is incompatible with the scientific propositions and models about molecular geometry and polarity. A student who possesses alternative conceptual frameworks such as JT often rejects the new information or generated misconceptions when he or she interprets the new information in his or her alternative conceptual framework. For the same reason, the student memorizes textbook explanations in pieces to deal with course exams. The fragmented knowledge has no foundation to be assimilated or reconciled upon. Thus the student loses the segments of knowledge in the memory soon after the exams.

General descriptions about conceptual frameworks. Based on the analysis of concept webs and observations of their interviews, students with low content knowledge had many missing conceptions as well as misconceptions, and other concepts were vague. These students frequently followed rules of thumb without understanding appropriate propositions behind these algorithmic approaches. These students held on to their algorithmic strategies and personal theories and did not reconcile these alternative strategies and conceptions with scientific explanations. While explaining a concept or a phenomenon, the links between/among concepts were missing or inconsistent. Also, their explanations had no supports or were justified with common sense explanations (e.g., teleological or anthropomorphic explanations).

The three students with low content knowledge had poor understanding about Bohr model, electron-cloud model, and quantum mechanics descriptions. They did not understand the meanings, explanatory power, or limitations of these models. Therefore, they predominately operated their thinking and solved problems based on 2D Lewis structures, but perceived the Lewis dot structures as verbal-linguistic representations. These students saw these structures as collections of letters, lines, and dots rather than conceptualizing the symbols as representations of atoms and molecules. The characteristics of students' conceptual frameworks for the high, moderate, and low content knowledge groups are summarized in Table 22.

Thinking with Mental Models – Interactions between Content Knowledge and Mental-Modeling Ability

Thinking based on a mental model is a dynamic interaction between an individual's content knowledge and mental-modeling ability. When constructing a mental model, an

Table 22

Conceptual Frameworks Comparisons for the High, Moderate, and Low Content Knowledge Students

	High content knowledge JS, RE, CR	Moderate content knowledge SD, AM	Low content knowledge JT, TA, KA
Atomic structure and representations of atomic models	• Considers effective core charge and its interaction with electrons (electrostatic force) • Bohr model with detail features o Associates electron shells with energy levels • 3D Electron-cloud model o Explains w/ quantum mechanic descriptions • Lewis dot structure	• Missing the influence of effective core charge and interactions of electrostatic force between the nucleus and electrons • Bohr model with only electron shell (nucleus is represented with a dot) (preferred) o Missing details o Possesses concept about electron shells but does not associate it with energy levels • 3D Electron-cloud model o Does not justify with quantum mechanic descriptions o Describes electron distribution as areas with electron-rich region and electron-poor region • Lewis dot structure	• Missing the influence of effective core charge and interactions of electrostatic force between the nucleus and electrons • Bohr model (missing details in the drawings) o Missing concepts about electron shells and energy levels • 2D Electron-cloud model (as a circle) o Does not justify with quantum mechanic descriptions o Incorrectly indicates electron distribution • Lewis dot structure (preferred)
Periodic trends	• Descriptions include numbers of total electrons and valence electrons • Descriptions include numbers of neutrons and protons • Electronegativity (justifies with electrostatic force) • Atomic radius (relates to the numbers of neutrons and protons) • Associates groups in the Periodic Table with reactivity and justifies with octet rule	• Descriptions include numbers of total electrons and valence electrons • Numbers of neutrons and protons were missing • Electronegativity (algorithm & memorizing, no justification) • Atomic radius (algorithm, no justification) • Missing description about reactivity	• Descriptions include numbers of total electrons and valence electrons • Numbers of neutrons and protons were missing • Electronegativity (algorithm & memorizing, no justification) • Atomic radius (algorithm, no justification) • Missing description about reactivity

Table 22

Conceptual Frameworks Comparisons for the High, Moderate, and Low Content Knowledge Students (continued)

(Continued)	High content knowledge JS, RE, CR	Moderate content knowledge SD, AM	Low content knowledge JT, TA, KA
Chemical bonding and the octet rule	• Chemical bonding is electrostatic force between two atoms • Octet rule - justifies with stability • Comfortable about exceptions of the octet rule	• Chemical bonding is some kind of attractive force between two atoms • Octet rule – justify with stability • Not comfortable about exceptions of the octet rule	• Chemical bonding is some kind of force between two atoms • Octet rule – justify with teleological explanations • Misconceptions about exceptions of the octet rule
Molecular shape and polarity	• RE and CR specifically use an idea of electron probability to explain polar bond (regions of devoid and dense of electrons) o Associates with electronegativity difference • Uses VSEPR model and justifies it with electrostatic force • Steps to determine geometry and polarity 1. Uses the VSEPR model to determine the arrangement of electron pairs in 3D 2. Applies propositions of direction of pulls (only CR used the term "dipole moment") to the 3D molecular structure then cancels out the pulls spatially and determines molecular polarity	• Uses an electron-cloud model to conceptualize polar bond as pulls of electrons o Associates with electronegativity difference • Vague use of VSEPR model and justifies it with electrostatic force • Steps to determine geometry and polarity 1. Uses the VSEPR model to determine arrangement of electron pairs in 3D OR Uses 2D Lewis structures to determine arrangement of electron pairs in 2D (for molecules with a novel geometric structure) 2. Applies propositions of direction of pulls (did not use the word "dipole moment") to the 3D structure then cancels out the pulls spatially and determines molecular polarity	• Explains polar bond as pulling of forces. Draws arrows to show its direction o Associates with electronegativity difference • Does not use VSEPR model. Frequently uses algorithm and 2D Lewis structures • Steps to determine geometry and polarity 1. Uses algorithm to determine molecular geometry or think about arrangement of electron pairs based on drawings of 2D Lewis structure 2. Applies propositions of direction of pulls (did not use the word "dipole moment") to a 2D or 3D molecular structure then cancels out pulls spatially and determines molecular polarity

Table 22

Conceptual Frameworks Comparisons for the High, Moderate, and Low Content Knowledge Students (continued)

(Continued)	High content knowledge JS, RE, CR	Moderate content knowledge SD, AM	Low content knowledge JT, TA, KA
Metacognition	• Reconciles conceptions in their conceptual frameworks	• Satisfies with partially accurate propositions, algorithm, and some personal theories • Does not reconcile disjointed conceptions and personal theories with conceptual framework	• Holds on to algorithmic strategies and personal theories • Does not reconcile disjointed conceptions and personal theories with their conceptual frameworks
General descriptions about conceptual framework	• Consists of precise, accurate conceptions; a few misconceptions or missing conceptions • Justifies their explanations with appropriate concepts • Conceptual framework is coherent • Switch between models o Different models connected and reconciled; sometimes has hybrid model o Models functional for explanation or problem-solving o Associates appropriateness of using model or representation with the context or problem	• Consists of accurate or partially accurate, but vague conceptions; a few misconceptions and some missing concepts • Only a few explanations supported; many concepts have no justifications or were justified with common sense reasoning (teleological or anthropomorphic explanations) • Conceptual framework is semi-coherent with some conflicting concepts • Switch between models o Different models not reconciled; indicates which model preferred, e.g. "pop-up in my head" o Models lose some power of explanation but still have power of illustration o Depends on which model is activated (or recalled) by the question	• Many misconceptions and/or missing concepts; other concepts vague and partially accurate • Many concepts have no justifications or justified with common sense reasoning (teleological or anthropomorphic explanations) • Conceptual framework is fragmented • Switch between models o Uses predominately 2D Lewis structure but perceives these structures as collections of letters, lines, and dots

individual is generating a 2D pictorial or 3D image based on his or her existing knowledge. Thus, accuracy and the level of details for the static/spatial features of a mental model reflect the individual's perceptions and/or comprehensions of a chemistry principle, representation, or a model. For example, CR, a student with high content knowledge, conceptualized the four lone pair electrons of a H_2S molecule as four probability regions of electron distribution overlapping each other. This feature of his mental model reflected his understanding about quantum mechanism descriptions. But SD, a moderate content knowledge student, adopted the image of hybridization of atomic orbital and misinterpreted the tear-drop shape of the electron probability regions as the space occupied by electrons. Thus, I consider that visualizing a mental model based on perceived information and/or existing knowledge is a type of interactions between content knowledge and mental-modeling ability.

Once the mental model is constructed and used to solve a problem, the individual needs to identify the context of the problem, choose the appropriate proposition to apply, and know how the proposition enacts on the model, then adjust the model accordingly to infer a potential answer. Therefore, I consider that the causal/dynamic mechanisms in a generated mental model and power of prediction and inference for these mechanisms indicate another type of interactions between an individual's knowledge and mental-modeling ability.

I analyzed the eight participants' mental models about H_2S and BF_3 molecules to verify interactions between quality of conceptual framework and the level of mental-modeling ability. Using grounded theory, a set of static/spatial features and causal/dynamic features emerged from the analyses that allowed me to categorize students' mental models. I assembled these features to form a protocol of mental models (Table 23) that I then used to recode and score the accuracy of static/spatial features and availability of causal/dynamic mechanisms of each participant's mental models. The scores of the spatial/static features illustrated whether the generated models and the student's explanations about the model containing correct attributes and spatial 3D information. The scores of the causal/dynamic features demonstrated how the students imposed appropriate propositions (e.g., the VSEPR model, electronegativity of each atom, and net dipole moment) to their mental model and were able to adjust their mental model accordingly. Each participant' mental models scores, based on the criteria outlined in the protocol of mental models, are reported in Table 23.

Table 23 shows that among the features of mental models about H_2S and BF_3 molecules, 6 out of 8 participants did not associate the arrangement of electron pairs for H_2S as a tetrahedral shape. Moreover, only JS conceptualized the bond angle mathematically according to the spatial information of a tetrahedral structure.
Table 24 illustrates the eight participants' scores of mental models about H_2S and BF_3 molecules in relation to their mental-modeling ability and level of content knowledge. Beside each participant, there are two numbers in each pair of brackets. The first number denotes the participants' score on mental-modeling ability (refer to the protocol of mental-modeling ability, Table 21), and the second number in the brackets indicates the participant' score based on the protocol of mental models (refer to the protocol of mental models, Table 23).

Participants' content knowledge determined the features of the mental model which included, but were not limited to attributes of lone pairs and bonds, numbers of bonding

Table 23

Protocol of Mental Models and Scores of Participants' Mental Models about H_2S and BF_3 Molecules

	Maximum Score	JS	RE	CR	AM	SD	TA	KA	JT
Spatial/Static features									
Lone pairs:									
PART: each lone pair consists of two electrons	*1*	1	1	1	1	1	1	1	1
ATTRIBUTE: Visualize electrons of lone pairs as a region of probability	*2*	2	2	2	0	1	0	0	0
Bonds (bonding electrons):									
PART: each bond consists of two electrons	*1*	1	1	1	1	1	1	1	1
ATTRIBUTE: Visualize electrons of lone pairs as a region of probability	*2*	2	2	2	0	1	0	0	0
Polar bonds:									
ATTRIBUTE: magnitude of bond dipole	*2*	2	2	2	2	2	2	2	1
SPATIAL RELATIONSHIP: directions of bond dipole	*2*	2	2	2	2	2	2	2	1
Arrangement of electron pairs in three dimensions:									
PART: Correct numbers of bonding pairs and lone pairs in a molecule	*1*	1	1	1	1	1	1	1	1
ATTRIBUTE: Relative radii of the atoms in a molecule	*1*	1	1	1	0	0	0	0	0
SPATIAL RELATIONSHIP (H_2S): arrangement of electron pairs – tetrahedral	*2*	2	0	0	2	0	0	0	0
SPATIAL RELATIONSHIP (H_2S): molecular geometry – bent	*2*	2	2	2	2	2	2	2	0
SPATIAL RELATIONSHIP (H_2S): bond angle (tetrahedral: 109.5°)	*2*	2	0	0	2	0	0	0	0
SPATIAL RELATIONSHIP (BF_3): molecular geometry – trigonal planar	*2*	2	2	2	2	1	0	0	2
SPATIAL RELATIONSHIP (BF_3): bond angle (trigonal planar: 120°)	*2*	2	2	0	2	2	0	0	2
Subtotal	*22*	22	18	16	17	14	9	9	9
Causal/dynamic features									
Electron repulsion exists among all bonding and lone pairs that determine									
a) molecular geometry	*2*	2	2	2	1	2	1	0	0
b) bond angles	*2*	2	2	2	2	2	0	0	0
Lone pairs have greater repulsion than bonding pairs	*2*	2	2	2	2	2	2	0	0
Bonded atoms will influence bond angles	*2*	2	2	1	1	0	2	0	0
Electronegativity difference determines direction and magnitude of bond dipole	*2*	2	2	2	2	2	2	2	1
Determine net dipole by balancing (or canceling) out dipole moments spatially	*2*	2	2	2	2	2	2	2	1
Determine whether the molecular is polar or non-polar based on its net dipole									
H_2S	*2*	2	2	2	2	2	2	2	0
BF_3	*2*	2	2	1	2	2	0	2	0
Subtotal	*16*	16	16	14	14	14	11	8	2
Total	***38***	**38**	**34**	**30**	**31**	**28**	**20**	**17**	**11**

and lone pairs, electronegativity of each atom, and propositions that the individual imposed on their mental model. The level of the participant's mental-modeling ability reflected his or her comprehension for the spatial information of a specific geometric structure; visualization of bond angle, directions of bond polarity, summation of net dipole moment based on a 3D geometry; and the degree of the connection between propositions and the structure of the mental model.

Table 24 suggests that there is a positive interdependent relationship between the level of content knowledge and the level of mental-modeling ability. For example, when the level of a student's mental-modeling ability was low, the quality of his or her conceptual frameworks was poor or vice versa. Among the eight participants, no students were observed as having high mental-modeling ability and low content knowledge, or low mental-modeling ability with high content knowledge.

Table 24

Participants' Scores of Mental Models in Relation to Their Mental-Modeling Ability and Level of Content Knowledge

	High content knowledge	Moderate content knowledge	Low content knowledge
High mental-modeling ability (7-10)	JS [10, 38] RE [10, 34]		
Moderate mental-modeling ability (3-6)	CR [6, 30]	AM [4, 31] SD [4, 28]	
Low/No mental-modeling ability (0-2)			TA [2, 20] KA [1, 17] JT [0, 11]

Based on my interview analyses, students having a high level of content knowledge and a higher level of mental-modeling ability were more accurate in spatial/static features of their mental model. Also, their mental models contained more causal/dynamic mechanisms available for prediction and inference. For students possessing lower level mental-modeling ability and lower level of content knowledge, their mental models lacked details of spatial/static features, and some causal/dynamic mechanisms were missing from their mental models.

Summary

This chapter first reported results of descriptive and inferential statistics. Second, it diagnosed misconceptions about molecular geometry, polarity, and prerequisite concepts using instruments EN, CB, and GP. The qualitative analyses included eight student interviews to identify students' mental-modeling ability, level of content knowledge, and features of their mental models. Based on the interview analyses, I categorized these eight students into high, moderate, and low groups in terms of their mental-modeling ability as well as their level of content knowledge. I reported characteristics of mental-modeling ability, conceptual frameworks, and features of mental models for each group. Cross-case analyses are discussed in Chapter Five.

CHAPTER FIVE

CONCLUSIONS AND IMPLICATIONS

This chapter includes a summary of the study, summary of both quantitative and qualitative study results, conclusions of findings for the quantitative phase, and assertions of findings for the qualitative phase. I also relate both conclusions and assertions to the research literature discussed in Chapter Two, and explain how this study contributes to the body of literature on student learning in chemical education. I conclude with implications for college chemistry teaching, research on student understanding, and suggestions for future research.

Summary of the Study

Research has shown that molecular polarity is a difficult concept for students to understand (Furió & Calatayud, 1996; Furió et al., 2000; Peterson et al., 1989); yet, literature focused on student understanding of molecular polarity is limited (Furió & Calatayud, 1996). It was this need that guided this study to investigate students' thinking processes on this abstract concept. The purpose of this study was to investigate student thinking processes while solving problems about molecular polarity. To answer the overarching research question: What are the influences on students' problem-solving about molecular polarity, I employed a mixed-method incorporating both quantitative and qualitative phases. Quantitatively, I collected student background information (gender and the number of previous chemistry courses) and their course performance (scores for exams 1, 2, 3, final exam, and course grade). Also, three diagnostic instruments EN (Taber, 2002b), CB (Jang, 2003; Peterson et al., 1989), and GP (Furió et al., 2000; Peterson et al., 1989), were used to gather information in terms of students' understanding and misconceptions about concepts of molecular geometry, polarity, and prerequisite concepts. Descriptive statistics and two one-way ANOVA were performed to analyze the relationships between gender, as well as the number of chemistry courses participants enrolled prior to Chemistry 1320 and their scores of the instruments EN, CB, and GP. The results of instruments EN, CB, and GP revealed several misconceptions of the student sample in the class to study.

To understand what contributes to the differences in students' understanding about molecular geometry and polarity, case studies were conducted on eight students who were sampled from the high-scoring (JS, RE, and CR), moderate-scoring (SD and TA), and low-scoring students (AM, KA, and JT) based on their scores on the three diagnostic instruments. Using a grounded theory, I preformed both within- and cross-case analyses using data from student interviews. Guided by the research questions, the qualitative findings were organized into three sections: students' mental-modeling ability, level of content knowledge, and the interactions between mental-modeling ability and content knowledge including features of mental models as outcomes of the interactions.

The eight cases were first analyzed to identify students' mental-modeling processes associated with spatial-thinking ability and other cognitive aspects that were not related to content knowledge. Four characteristics emerged from the interview analyses portraying a sophisticated mental-modeling process when solving a molecular polarity problem. These four characteristics were assembled to form a protocol (refer to Table 21) that was later used to recode and score the eight participants' mental-modeling ability. Based on their scores, the eight students were then assigned to one of the three mental-modeling abilities: high (HMMA), moderate (MMMA), and low mental-modeling ability (LMMA) groups.

Next, I examined students' explanations, along with their models and drawings, to explore their level of content knowledge. I started coding the videos with the high-scoring students for key concepts and subsequent concepts, and used high-scoring students' conceptual frameworks a criterion for cross-case comparisons. I then recoded each interview in order to verify or modify the elements and links to the initial webs to best represent the participant's conceptual framework. Three concept webs were developed to analyze each student's conceptual frameworks about (1) atomic structure, periodic trends, and representations of atomic models, (2) chemical bonding and the octet rule, and (3) molecular geometry and polarity. Based on the quality and content of their conceptual frameworks, I categorized the eight participants as having high, moderate, or low content knowledge groups.

The eight participants' mental models about H_2S and BF_3 models were then analyzed regarding the accuracy and level of details of spatial/static features for their mental models, as well as whether the individuals imposed appropriate propositions to the causal/dynamic features of the models. I developed a protocol of mental models with features which emerged from the interview analyses, and used it to code and score each student's models. These scores were then interpreted in light of the individual's interactions between mental-modeling ability and level of content knowledge.

Summary of Findings

Quantitative Results

The quantitative results involved data from 159 students. The results of one-way ANOVAs indicated that there were no statistically significant differences for the mean scores between male and female students on scores of instruments CB and GP, exams 1, 2, and 3, the final exam, and the course grade. Only on instrument EN did male students score significantly higher than scores of female students. The correlation coefficients indicated that the scores on instrument EN had only a weak correlation with scores on instruments CB, GP, as well as on exams 1, 2, and 3, the final exam, and the course grade. One possible explanation for the weak correlation for instrument EN with scores on other instruments and exams was that concepts about electronegativity, addressed by instrument EN, are associated and conceptualized by students in terms of propositional statements. Other concepts such as chemical bonding, molecular geometry, and polarity assessed by instruments CB, GP, and course exams were involved construction of mental models and visualization skills. The nature and format of the knowledge stored in an individual's conceptual framework may contribute to the weak correlation among scores on the diagnostic instruments and exams. Scores on both instruments CB and GP had a moderate correlation with the four course exams and course grade. Also, the results of one-way ANOVA showed that the effect of the number of previous chemistry courses students was not statistically significant for students' scores on instruments EN, CB, and GP, the four course exams, or the course grade.

Results of instrument EN indicated that more than half of the students in this study were committed to misconceptions including alternative notions of stability, an alternative electrostatic principle – conservation of force, and applying Coulombic principle. Other misconceptions identified by instruments CB and GP involved chemical bonding, bond polarity, molecular shape, and molecular polarity. Among these misconceptions, alternative notions of stability followed by conservation of force were commonly shared among the students.

Qualitative Results

Findings on students' mental-modeling ability showed that the level of mental-modeling ability can be thought of as a continuum with the LMMA group representing students who do not have or have very limited ability to generate and use mental models, as opposed to the HMMA group which demonstrated a sophisticated ability to both constructing and using mental models. In addition, HMMA students constantly evaluated their mental models and monitored their mental-modeling processes.

Examining students' content knowledge indicated that the high content knowledge students' conceptual frameworks were coherent and consisted of precise, accurate conceptions with only few misconceptions, missing conceptions, or missing links. Their coherent conceptual frameworks allowed the high content knowledge students to justify their explanations with appropriate concepts, reconcile new information easily, and switch between models with little difficulty based on the content of a problem. In contrast, conceptual frameworks for students in the low content knowledge group were fragmented and contained many missing concepts, missing links, and/or misconceptions. The students with fragmented conceptual frameworks could neither reconcile different models and disjointed conceptions, nor supplement appropriate propositions to construct a functional 3D mental or concrete model with accurate spatial features. Instead, low content knowledge students predominately used 2D Lewis structures to solve a problem. Because their conceptual framework and pieces of knowledge were not effective to solve a problem, these low content knowledge students held on to algorithmic strategies and personal theories. In addition, they could not justify their explanations or justified them with common sense explanations.

The analyses of features of students' mental models suggest a positive interdependent relationship between an individual's content knowledge and mental-modeling ability. For example, students having a high content knowledge and a higher level of mental-modeling ability were more accurate in spatial/static features of their mental models. Their mental models contained more causal/dynamic mechanisms that enabled them to make further predictions and inferences. On the other hand, for students possessing lower level mental-modeling ability and lower level of content knowledge, their mental models lacked details of spatial/static features, and some causal/dynamic mechanisms were missing from their mental models.

Conclusions and Assertions

Results of diagnosed misconceptions in the quantitative phase and the comparisons of the eight selected students' mental-modeling ability and content knowledge are discussed in this section. Additionally, I compare the findings of this study with the research literature to understand how the findings from this study help to fill gaps in the literature or provide a different perspective. To organize this section, I follow the same structure as in Chapter Four, beginning with conclusions for findings of the quantitative phase followed by assertions of case analyses for mental-modeling ability and content knowledge. At the end, I discuss the interdependent relationship between students' content knowledge and mental-modeling ability.

Conclusions for the Quantitative Phase

Conclusion 1. Comparing common misconceptions identified in the current study with previous literature. Percentages of students possessing misconceptions (Table 11 and 14) identified by instruments EN, CB, and GP were similar to the findings in the original studies on most items. Only on five items about alternative notion of stability, applying Coulombic principle, and chemical bonding were the percentages of incorrect responses in the current study considerably higher than in the original studies (see Table 25). The three items categorized as alternative notion of stability indicated that more students committed to the octet rule in the current study than the UK students in Taber's study (2003b).

Conclusion 2. When the concept to be tested involves (a) comprehension of a generic structure in 3D and of propositions or (b) multiple logic steps to derive the answer, the current design of diagnostic instruments may not be an effective tool to analyze students' understanding. The use of three diagnostic instruments in the quantitative phase allowed me to gather information about students' understanding of the prerequisite concepts for a large student samples in a short period of time. The three diagnostic instruments adopted in this study were grounded in literature and provided interviews focusing on students' misconceptions. In addition, these diagnostic instruments were individually validated on large student samples with reliability. Thus, the comparisons of students' responses to the diagnostic test items and interviews confirmed that the test items were effective in diagnosing students' misconceptions about

Table 25

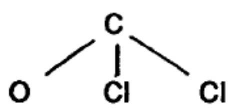
Comparing Common Misconceptions Identified in the Current Study with Previous Literature

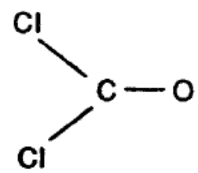
	Current study Incorrect %	Original study Incorrect %
Alternative notion of stability (Taber, 2003b)		
EN-12. If the outermost electron is removed from the atom it will not return because there will be a stable electronic configuration.	77%	52%
EN-4. Only one electron can be removed from the atom, as it then has a stable electronic configuration.	59%	24%
EN-3. The atom will spontaneously lose an electron to become stable.	32%	14%
Applying Coulombic principle (Taber, 2003b)		
EN-6. Each proton in the nucleus attracts one electron.	55%	27%
Chemical bonding (Jang, 2003)		
CB-6. After sodium atom donates its valence electron to the chloride atom, the sodium ion forms a molecule with the chlorine ion	33%	17%

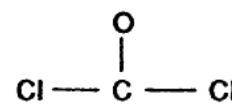
electronegativity and chemical bonding. However, I found that students' responses to the test items regarding molecular geometry and polarity sometimes showed conflicting results between different items and/or did not always correspond to students' interview responses.

A possible explanation is that electronegativity and chemical bonding concepts involve mostly declarative knowledge. When students responded to the items on concepts of electronegativity and chemical bonding, the items were assessing propositions that students used to justify their answers. However, solving problems about molecular geometry and polarity successfully requires students to not only apply appropriate propositions, but also to visualize a geometric structure with correct spatial information. Diagnostic items in a paper-and-pencil format, or implemented electronically as in the current study, could only represent a molecular structure in 2D. With this limitation, the diagnostic items may not be effective in distinguishing whether students' incorrect responses were due to them not having appropriate understanding of chemistry principles or due to their inability to visualize the 3D geometric structure of the given molecule of the item. One example is item GP-5 (see Figure 40):

Which of the following best indicates the shape of the $COCl_2$ molecule?

(1) 

(2) 

(3) 

<u>Reason</u>

(A) The shape of the $COCl_2$ is dependent on the electronegativity of each atom.

(B) The shape of the $COCl_2$ is due to approximately equal repulsion between the bonding and non-bonding electron pairs on the carbon.

(C) The shape of the $COCl_2$ is due to the stronger polarity of the C=O double bond in the molecule

(D) The shape of the $COCl_2$ is due to equal repulsion between the bonding regions formed by the atoms joining to the carbon.

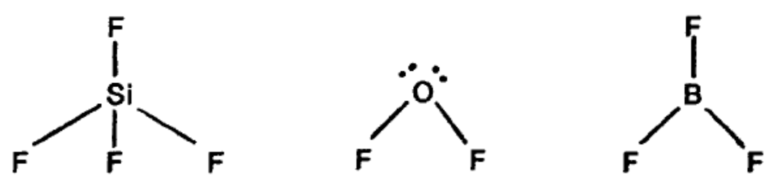
Figure 40. Instrument GP, item 5.

SD chose an incorrect answer (3) in the first tier and a wrong reason for the second tier (B). Based on her interview responses while solving a problem about BF_3, I found that SD understood the VSEPR model and could draw a correct Lewis structure. However, she had a difficulty visualizing a trigonal planar shape; therefore, she tended to draw the initial structure in a T-shape and wondered whether she should fill the void on the Lewis structure with a lone pair. For a case like this, the diagnostic item was not able to determine whether her erroneous response was due to not being able to construct a correct Lewis structure or due to her inability to visualize the geometric structure in 3D.

Also, HMMA and LMMA students used 2D Lewis structures for different visual cues, depending on whether the molecule had a familiar geometric structure or not. Therefore, students' responses to an item with a molecular structure that they have seen frequently may be different from the response to an item with a novel molecule.

Another possible explanation is that solving problems about molecular geometry and polarity successfully requires students to work through multiple steps of reasoning and to consider multiple conditions of a problem. Students may have selected the most significant feature or a condition of the problem that came to their mind when responding to the reason part of the item (see item GP-2 in Figure 41).

Which one of the following molecules is polar?



(1) (2) (3)

Reason

(A) The polarity of the molecule is due to the high electronegativity of fluorine.

(B) Non-symmetrical molecules containing atoms of differing electronegativity are polar.

(C) Non-bonding electrons on an atom in the molecule produce a dipole and hence a polar molecule.

(D) A large difference in the electronegativities of the atoms involved in bonding results in a polar molecule.

Figure 41. Instrument GP, item 2.

SD chose the correct answer (2) in the first tier, but a wrong reason (C) in the second tier and thought that OF_2 was polar because the non-bonding electrons produce a dipole.

After discussing the H_2S molecule problem with her in the interview, I found that SD understood and considered both the geometric structure of the molecule and the electronegativity difference when determining molecular polarity. It is possible that SD chose reason (C) for this question because the two lone pairs were the significant feature of the OF_2 molecule, and she was aware that the lone pairs would result in an electron-rich region in the OF_2 molecule. This first impression about lone pairs clouded SD's actual understanding from being identified by the diagnostic item. When the concept to be studied involves multiple logic steps to derive the answer, the current two-tier design of diagnostic items may not be as effective as for concepts that require only a single logic step. The effectiveness of using diagnostic items on this type of concepts has not been discussed in the previous literature.

Conclusion 3. Diagnostic instruments indicated the actual level of students' understanding about molecular geometry, polarity, and prerequisite concepts better than the course exams. Results of this study showed that diagnostic test items are effective in eliciting students' misconceptions regarding concepts about electronegativity and chemical bonding. This study used students' scores on their diagnostic instruments to classify students into high-, moderate-, and low-scoring groups, and the results showed that only AM and TA were improperly classified. Therefore, AM was relocated from the low-scoring group to the moderate content knowledge/MMMA group, and TA was reassigned from the moderate-scoring group to the low content knowledge/LMMA group. Comparisons of interviewed participants' responses to the diagnostic test items and interviews suggested that students' scores on the three diagnostic instruments reflected students' understanding about molecular geometry and polarity. The design of the two-tier diagnostic items forced students to justify their reasons; therefore, diagnostic items contained greater power to elicit students' understanding. Here I quote SD's comments on the two-tier diagnostic items to support my argument about why the diagnostic instruments have a greater diagnostic power compared with traditional test items:

> It is really funny because when I was going through and doing the concept things [two-tier diagnostic instruments]… I'd get the answer right and then the explanation was wrong, and I was like "how do I do that"? It is not a guess, it is my own little method but it does not work when you try to explain it….Yeah I'd try to like pick the one that fit mine the most. Sometimes I do not know exactly what the term is that I'm using to figure it out. So it is harder that way, because it is like you're explaining what you're doing. [When the Blackboard system provided the answers,] for me it [the answer for the first tier] makes sense. The explanation did not make sense. I was like, "that's not the way to say it." I could not figure out what that would be, so I just would put what was closest to how I would say it and that I would be wrong. (SD, interview)

SD indicated that she applied her own theories to choose an answer that matched her explanations the most in the reason part. After the answer keys were provided, she was surprised that her personal theories that often gave her correct answers were indicated as wrong explanations.

When comparing students' scores on the diagnostic instruments to their course performance (Table 26), diagnostic instruments showed to be more accurate in assessing the actual level of students' understanding about molecular geometry and polarity. A possible explanation for students' course performance is that moderate and low content knowledge students may use their personal theories, algorithmic strategies, and/or rote memorization to survive through the course examinations.

Table 26

Level of Content Knowledge, Mental-Modeling Ability, and Course Performance for the Eight Interview Participants

Participants (rank of scores based on EN, CB, and GP)	Content knowledge	MMA	Exam1	Exam2	Exam 3	Final	Course grade
JS (high-scoring)	High	High	95	90	90	93	93.6
RE (high-scoring)	High	High	80	90	55	71	77.6
CR (high-scoring)	High	Moderate	100	100	90	96	99.3
SD (moderate-scoring)	Moderate	Moderate	75	65	65	62	74.4
AM (low-scoring)	Moderate	Moderate	80	80	65	84	83.8
TA (moderate-scoring)	Low	Low	65	85	70	73	81.1
KA (low-scoring)	Low	Low	70	80	70	87	86.8
JT (low-scoring)	Low	Low	80	75	65	89	84.6

Assertions on Comparisons of Students' Mental-Modeling Ability among the HMMA, MMMA, and LMMA Groups

Assertion 1. Both HMMA and MMMA students performed visualization skills to generate and operate a 3D mental model. These visualization skills were not observed in LMMA students. The LMMA students relied on drawings of 2D Lewis structures for inference and reasoning. Visualization skills are essential for students to comprehend 3D molecular geometry and to understand concepts involving 3D spatial information such as molecular polarity. In this study, the observed visualization skills included: understanding accurately a 3D object from its 2D representation (spatial visualization), imagining what a representation will look like from a different angle in 3D (spatial orientation), and visualizing effects of operations such as rotation, or mentally manipulating the object (spatial relations). Due to the design of interview questions, students in the current study did not demonstrate all the visualization skills indicated in

Ferk et al.'s (2003) study. In the following quote RE explains how she used visualization skills to transform a 2D Lewis structure of a carbon tetrachloride (CCl_4) molecule into a 3D mental model to understand its molecular polarity.

> If I want to think about the shape of a tetrahedral molecule, I can see that in my head. I see it basically as a model with straws or sticks and little balls. I can see how it is and I can have it turn and move around in my head. For awhile I pictured it in my head like the Lewis structure, like this [Figure 42]. And I thought, well that must be a polar molecule because these three are all pulling down, and this one is pulling up, so that's only canceling out this one [the pull pointing downward]. But then, when I learned that all the angles are 120°, I had to picture it in my head and flip it upside down and turn it around, and see that it was all even on all the sides and the pull is going in all this opposite directions [15:52-16:50] (RE, interview)

Figure 42. RE's drawing of a CCl_4 molecule.

On a different note, SD described her experience with simulation software in laboratory as useful in helping her to incorporate rotation into her ability to visualize.

> In my mind I could turn it [H_2S] and look at it from a different angle because we did those computer things in our lab, where we did it on a computer, and so I got used to turning them around on that. So I kind of integrated that into my little flat screen descriptions I had in my head. So I look at it in different ways, but I mean, I understand that it can turn and it looks different from a different angle, but essentially it is still always going to look relative [same arrangement of electron pairs] in my head. [16:01-17:08] (SD, interview)

Visualization skills were reported by HMMA and MMMA students, but not by LMMA students when solving problems of molecular polarity. It is important to clarify that LMMA students in this study did possess some mental-modeling ability. For example, JT visualized electrons moving around the nucleus of a sulfur atom like the solar system. However, when solving problems about molecular geometry and polarity, JT relied on a 2D Lewis structure and did not apply his visualization skills to the molecular structure. LMMA students' reliance on 2D Lewis structures for inference and reasoning often resulted in wrong answers. This could be because the 2D Lewis structure loses the depth of spatial information; therefore, the 2D Lewis structure does not facilitate inference and reasoning spatially (Wu & Shah, 2004). For some students in the MMMA and LMMA groups (e.g., when TA solved a problem about polarity of BF_3), when a concrete model that represented accurate spatial information in 3D was used, it increased their ability to infer a correct answer, but only if the propositions applied to the model were correct.

Assertion 2. 2D Lewis structures provided two types of visual cues for a student to construct a mental model. The students' level of mental-modeling ability and their familiarity with the geometric structure of the given molecule determined the type of visual cues the student used. Students in the HMMA group constructed a 3D mental model of a given molecule by forming and labeling imaginary atoms without drawing a 2D Lewis structure. Simultaneously, these students accounted for the numbers of bonds and lone pairs so they could then apply the VSEPR model to arrange the relative position of each atom and determine its 3D molecular geometry. For molecules not frequently seen in the textbook or lectures, the HMMA students drew a 2D Lewis dot structure either prior to the mental model construction or at the end, as a means of verifying their mental model. For most students in the MMMA and LMMA groups, drawing a 2D Lewis dot structure of a given molecule was a necessary step before the mental model could be generated.

For students in the HMMA and MMMA groups, a 2D Lewis structure provided cues about numbers of bonds and lone pairs in the molecule to ensure the constructed 3D mental model contained sufficient features to apply the VSEPR model and then use it to determine its geometry. Students in the LMMA group either used the cues of numbers of bonds and lone pairs in the Lewis structure to recall a stored mental image of 3D molecular geometry algorithmically, or directly used the 2D Lewis structure as a visual cue to generate a similar mental model. For a molecule the student had seen frequently and perhaps had memorized, a LMMA student could recall its 3D geometric structure algorithmically. If the molecule was unfamiliar however, MMMA and LMMA students would employ the 2D Lewis structure as a basis for inferring and reasoning.

These two assertions about LMMA students' difficulties in constructing mental models support findings from previous studies that most of secondary students were unable to identify the depth cue of 2D model (Seddon, Eniaiyejy, & Chia, 1985) or form 3D mental image by visualizing 2D structures (Tuckey, Selvaratnam, & Bradley, 1991).

Assertion 3. Three types of knowledge may influence students' ability to manipulate mental models based on an imposed proposition (characteristic 2). This characteristic is crucial for incorporating an individual's content knowledge with his or her visual-spatial thinking ability. The ability to manipulate a mental model while applying propositions to the model (characteristic 2) is crucial to solving a problem (e.g., a problem about molecular polarity) that involves both chemistry principles in propositional descriptions and spatial information of molecular geometry. This characteristic in the protocol of mental-modeling ability is also an important ability for incorporating the individual's content knowledge with his or her visual-spatial thinking ability. This characteristic helps the students comprehend how a chemical principle affects the structure of a 3D object, such as why the VSEPR model can be used to predict a molecular structure.

Students in the HMMA group were able to manipulate their mental models as tools of thinking for making inference and justifying their adjustments to the model with appropriate chemistry principles. Students who had a low score on the second characteristic of mental-modeling ability (see Table 21) generally concluded that the structure of their mental model would not change when adding an additional condition to the mental model, such as replacing two hydrogen atoms in a H_2S molecule with two chlorine atoms. Wu and Shah (2004) described that students with high spatial ability tend to perform better on chemistry tasks because they are able to mentally manipulate information in 3D or represent complex information visually. The comparison of students' mental-modeling ability provides direct evidence to support Wu's and Shah's conclusion.

Analyses of the interviews showed that three types of knowledge may have influenced the students' ability to manipulate mental models based on an imposed proposition. These types of knowledge are

1. The student's comprehension of the molecule's 3D molecular geometry, so he or she can visualize its structure spatially.
2. The student's existing knowledge of chemistry principles (e.g., the principle of electrostatic force, the VSEPR model) that determine the spatial arrangement of electron pairs.
3. The student's ability to connect chemistry principles to the spatial structure of the molecular geometry.

Evidence showed that missing any of the three types of knowledge could hinder a student's ability to manipulate mental models.

Assertion 4. Metacognitive actions (characteristic 3 and 4) are critical for successful mental-model reasoning. HMMA students performed a series of metacognitive actions throughout the mental-modeling process, but these actions were not observed for some MMMA students or any LMMA students. HMMA students applied metacognition throughout the mental-modeling processes and used an alternative approach to verify their mental model at the end to address any uncertain steps or answers. HMMA students' metacognitive actions included (1) recognizing context and conditions of a problem, (2) overseeing the processes of mental model construction to ensure the constructed model contained accurate features and spatial information to solve the problem, and (3) recognizing their approaches and monitoring steps of mental-modeling, as well as quality and accuracy of their knowledge to apply to the mental model.

These metacognitive actions were not demonstrated by some MMMA students or any LMMA students. The MMMA and LMMA students failed to recognize the mistakes of their mental model and/or steps of using mental or concrete models to solve a problem. Sometimes these students suspected or recognized that their mental model or knowledge was incorrect, but had no actions to reconcile or correct their errors.

Monitoring the mental-modeling process metacognitively (characteristic 3) would reduce the possibility of missed steps or neglected considerations of the proposition(s) during the problem-solving processes. It would also help to identify the conditions of a problem for the purpose of determining whether the constructed mental model contains sufficient features for solving the problem. In addition, self-checking using an alternative approach (characteristic 4) could also lead students to identify and correct errors at the end of the mental-modeling process. These two characteristics of metacognition resulted in students' thinking processes to have minimum of errors. The students also gained more confidence of their answers derived from their mental models.

The review of literature in Chapter Two summarized four learning impediments at the submicroscopic-symbolic domain: lack of appreciation about role of models, abstraction and unfamiliarity with symbols, difficulty with shifting between/among chemical representations, and a low visual-spatial thinking ability reported in chemistry education literature. Metacognition was not discussed in literature on mental-modeling ability. This study has provided evidence showing that metacognition plays a critical role for solving problems with mental model successfully. Thus, future research should consider metacognition when studying students' mental-modeling processes.

Assertions on Comparison for Levels of Content Knowledge among High, Moderate, and Low Content Knowledge Groups

Table 22 summarized characteristics of students' conceptual frameworks for the high, moderate, and low content knowledge students. Based on cross-case analysis of the conceptual frameworks, I generated five assertions.

Assertion 1. All participants justified the formation of chemical bonds and a chemical compound with the octet rule. Only two students, JS and CR, associated bond and chemical compound formation with the interactions of electrostatic force among atoms. Among the eight interviewed participants, six students merely followed the octet rule as a rule of thumb without understanding the chemistry principle behind the octet rule. The octet rule was a common misconception held by the interviewed participants.

Five out of eight interviewed students responded to at least 4 out of 5 items incorrectly for questions involving the octet rule on instrument EN. Interview analyses of moderate and low content knowledge student showed they followed the octet rule without understanding the chemistry principles. This hinders students from considering criteria and restrictions when using the octet rule to determine a Lewis structure for a given molecule.

Talanquer (in press) considered this line of thinking as teleological reasoning, where students considered "filling the octet" as the driving force for forming a chemical compound. Talanquer also indicated that many sources of students' teleological explanations were from the textbook or classroom instructions. For example, teleological statements were found in the textbook used in course:

> The formation of these molecules illustrates the *octet rule: An atom other than hydrogen tends to form bonds until it is surrounded by eight valence electrons* (italics in original). In order words, a covalent bond forms when there are not enough electrons for each individual atom to have a complete octet. By sharing electrons in a covalent bond, the individual atoms can complete their octets. …When an atom of one of these elements [in the second period in the periodic table] forms a covalent compound, it can attain the noble gas electron configuration [Ne] by sharing electrons with other atoms in the same compound. (Chang, 2005, p.355)

According to Talanquer's (in press) findings, I should not be surprised that the participants possessed these teleological explanations about the octet rule. He explained that at the general chemistry level this may be an appropriate pedagogical approach to introducing a concept without going into complex explanations.

Once the octet rule is perceived by a student as the explanation for why atoms share or transfer electrons to form chemical bonds or a chemical compound, it is difficult for students to reject the rule and reconcile it with other scientific explanations. However, among the eight participants in this study, only JS and RE partially reconciled the notion of the octet rule with principles of electrostatic force while thinking about chemical bonding. For example, when JS was asked about why a molecule would prefer to meet the octet rule, he replied, "It is about stability is what I've always been taught. And I guess I've been working off just trusting and then not really understanding if an orbital is more stable" (JS, interview). This example demonstrates how JS simply accepted what he had been taught; that a full or a half-filled orbital is more stable without really understanding why. Teleological explanations, such as those found in the course textbook, leave a void in students' thinking and reasoning when developing conceptual frameworks.

Assertion 2. Three key concepts need to be addressed in order to learn concepts about molecular shape and polarity successfully: a) the concept of atomic structure, b) the concept of effective core charge and principles of electrostatic force, and c) quantum mechanics descriptions. Concept web analyses of students' explanations across three levels of content knowledge allowed me to study how missing prerequisite concepts or linkages among conceptions, partial or incorrect understanding, or fragmented conceptions may result in misconceptions or failure of learning. The results of comparisons indicated that students in the low content knowledge group did not understand concepts of atomic structure and perceived atoms as Lewis structures. They perceived a fluorine atom as a letter surrounded by seven dots representing seven valence electrons. Due to not understanding atomic structure, these students could not describe the similarities and differences between a fluorine and a chlorine atom and merely replaced the letter F in the center of a Lewis dot structure replacing it with Cl to represent a chlorine atom. Marais and Jordaan (2000) indicated that first year chemistry students had more difficulty with meanings of symbols than with the meanings of words.

Indeed, symbols are the most abstract chemical representations, and students need to understand the entities that the symbols mean to represent before they can master the use of symbols. Cokelez and Dumon (2005) reported that 34% and 30% of French Grade 12 students preferred using symbols with Lewis dot structure or a simple sphere, respectively, to represent an atom. However, 75% of Grade 12 students did not use or provided erroneous answers while using a more abstract model to represent an atom. Only 10% of Grade 12 students indicated a model of neutral atom (where the number of protons equals the number of electrons). Cokelez's and Dumon's findings suggest that the concept of atomic structure needs to receive more attentions from college chemistry instructors.

The role of effective core charge and principles of electrostatic force were the second set of key concepts missing from the conceptual frameworks for students in the moderate and low content knowledge groups. Students in the moderate content knowledge group had a basic understanding about atomic structure, with the nucleus in the center and electrons surrounding on the outside. However, the influence of effective core charges and the nucleus-electrons interactions were missing from their conceptual frameworks. The moderate content knowledge students understood neither the relationships between numbers of protons and of electrons, nor associate levels of electron shells with energy levels. Missing the concepts of the nucleus-electrons interactions in an atomic model and the magnitude of energy involved may have hindered these students' comprehension about differences and similarities between elements (e.g., electronegativity, atomic radius), which generalize the periodic trends across groups and periods in the Periodic Table.

The missing role of the effective core charge may result from a pedagogical reason. Taber (2003) indicated that some high school chemistry teachers in the UK considered the content of electrostatic force to be too abstract for use in chemistry. Thus, these teachers used descriptive statements, such as "there is a force between the nucleus and electrons" to describe the nucleus-electrons interactions without referring to the basic physical principle pre se (e.g., $F \propto q_1q_2 / r^2$).

Missing the concept of nucleus-electrons interaction and principles of electrostatic force may have a profound influence on students' understanding of more advanced concepts. Based on my interview analyses, students who lacked understanding of the effective core charge could not articulate the principle of electrostatic force and perceived the periodic trends as rules of thumb or segments of facts, which they may eventually forget. Also, they described chemical bonding as some kind of attractive force between two atoms, but could not associate bonding with the electrostatic force between nuclei and electrons of the two atoms. Due to this lack of understanding about effective core charge, these students used word association to conceptualize covalent bonding and thought that covalent bond means to share electrons without considering the attraction from the nucleus of a more electronegative atom.

Thus, I propose that insufficient understanding about the concept of effective core charge and principles of electrostatic force hindered students' conceptualization about electronegativity and chemical bonding (both covalent bonding and ionic bonding), and possibly enhanced the overgeneralization of the octet rule when developing a Lewis structure of a molecule.

Quantum mechanics descriptions was the third key concept missing from conceptual frameworks for students in the moderate and low content knowledge groups. Moderate content knowledge students relied on an electron-cloud model while thinking about concepts of polar bond and the VSEPR model. Low content knowledge students perceived a molecule with a ball-and-stick model or a Lewis structure, and the lone pairs were omitted from the molecular structure. Both moderate and low content knowledge students had difficulties conceptualizing lone pairs of atomic orbital hybridization as probability regions of electron distribution and misinterpreted an electrostatic potential map as an area of electron distribution. The analyses of students' explanations suggested that students were not able to develop precise and accurate understanding about the VSEPR model unless their concepts about quantum mechanics and hybridizations of atomic orbital were resolved.

Taber (2001b) argued that students' conceptual development is a gradual shift of the preferred choice among several alternative explanatory principles (or models) as chemistry students progress through academic levels and are exposed to more sophisticated models. Students may simultaneously hold manifold explanatory conceptual schemes for a particular concept. Over time, when students undergo conceptual revolutions, their cognitive structure comes to favor the growth of a new alternative scheme that has more explanatory power (e.g., Coulombic forces) over the naïve idea (e.g., octet rule).

Assertion 3. Levels of students' content knowledge can be considered as a continuum. On one end, students possessed coherent conceptual frameworks composed of precise and accurate concepts. When moving to the other end, students' conceptual frameworks became fragmented with many misconceptions and missing concepts. Along the continuum from high level to low level of content knowledge, the quality of students' explanations declined, as did their ability to reconcile new information to their existing knowledge framework. Low content knowledge students' low quality and fragmented concept frameworks were related to their use of algorithmic strategies and common sense explanations while solving a problem. However, the direction of this relationship remains unclear. High quality of conceptual frameworks are characterized by more accurate and precise concepts, less misconceptions and missing concepts, and concepts that are connected with appropriate links. When the quality of students' conceptual frameworks decreases, the quality of students' explanations for a concept or a phenomenon declines. My analysis students' conceptual frameworks indicated that students with high levels of content knowledge justified their explanations with appropriate concepts. Students in the moderate content knowledge group often supported their explanations with vague propositions or sometimes had no justification. Low content knowledge students, who had fragmented conceptual frameworks with misconceptions and missing concepts, used algorithmic strategies without justification or supported their explanations with personal theories or common sense explanations.

I also found that students with high quality conceptual frameworks assimilated and reconciled new information consistently with their existing knowledge. For students in the moderate and low content knowledge groups, key concepts that anchored the new information to their conceptual frameworks were missing, or the new information was incompatible with their personal theories. Thus, these students experienced greater difficulties reconciling new information with their conceptual frameworks.

While analyzing students' content knowledge and quality of explanations, low content knowledge students' algorithmic strategies and common sense explanations are worth special attention. Common sense explanations are explanations about a natural phenomenon that individuals develop based on intuition and broad generalization, or shortcuts of reasoning procedures that learners learn from experience to make inferences with less effort (Talanquer, 2006). Based on my interview analyses, high content knowledge students used algorithmic strategies on occasion, but closely associated these strategies with the underpinning chemistry principles. Moderate content knowledge students more often used algorithmic strategies and justified these strategies with common sense explanations (teleological or anthropomorphic explanations) when their low quality of understanding for related principles was unable to support their explanations.

For some low content knowledge students, using algorithmic strategies was a habit of thinking, like what KA indicated in the interview: "I do not think I've ever thought of this so conceptually before. I just seem to plug it on and try it" (KA, interview). KA's satisfaction with his algorithmic strategies may have hindered him from devoting extra efforts to reconcile his disjointed knowledge. Different from KA's algorithmic approach, JT's failure to solve problems about molecular shape and polarity resulted from his thinking with personal theories. Because his conceptual frameworks were fragmented, JT developed personal theories to fill the gap between concepts or directly connected whatever concepts came to his mind at the moment.

Furió and Calatayud (1996) and colleagues (2000) used multiple-choice questions and two open-ended items to study Grade 12, first year, and the third year university chemistry students' concepts about molecular geometry and polarity. They attributed students' errors on solving molecular geometry and polarity problems to procedural difficulties. Procedural difficulties occur when students fail to solve a problem due to their reduction of the intrinsic complexity of the problem (functional reduction) or due to their use of common sense explanation with out considering the scientific knowledge (functional fixedness).

Findings from my interview analyses showed that students' errors in solving molecular geometry and polarity problems could result from possessing their personal theories, relying on algorithmic strategies, or possibly, procedural difficulties. However, a common point shared among low content knowledge students was their fragmented conceptual frameworks with many missing concepts, missing links, and misconceptions.

Assertion 4. Students with high content knowledge possessed precise and accurate concepts about atomic and molecular models that supported reconciliation among models. The reconciliation among models permitted these students to shift among models with minimum difficulty during problem-solving processes. Students in the moderate and low content knowledge groups had insufficient understanding about atoms and molecules which hindered their reconciliation among models. Thus, these students preferred a simple model or the one that they were most familiar with when solving a problem. Precise and accurate concepts about atoms and molecules support reconciliation among models. With sufficient understanding about meanings, explanatory powers, and limitations of the atomic and molecular models, students in the high content knowledge group were able to identify the context of a problem and choose an appropriate model. Also, because their understandings about models were reconciled and tightly connected, these students could switch between models easily as need for explanations. For example, students in the high content knowledge group used simple Lewis structure or a ball-and-stick model when they knew that the simple representation contained enough information to solve the problem. When the simple representation was unable to explain a phenomenon, such as to explain the electron distribution of a polar bond, they could switch to an electron-cloud model or quantum mechanics descriptions with no observable difficulties. This observation aligns with findings of Coll's and Treagust's (2001) study on Grade 12, undergraduate, and postgraduate Australian students' mental models of chemical bonding.

When the quality of students' understanding about models decreased, the insufficient understanding hindered moderate and low content knowledge students' reconciliations among these models. For the same reason, models lost their power of explanation or prediction when these students used the models during problem-solving processes. Due to their incomplete understanding about models, these students preferred a simple model or one that they were most familiar when solving a problem. For example, students in the low content knowledge group used the model "pop-up" in their mind when the given question triggered a specific model. Also, the low content knowledge students predominately tended to think about and solve problems based on 2D Lewis structures. They perceived the Lewis dot structures as verbal-linguistic representations and viewed these structures as collections of letters, lines, and dots rather than conceptualizing the symbols as representations of atoms and molecules. This observation of low content knowledge students echoed Shane's and Bodner's (2006) findings about general chemistry students' understanding of the relationship between the structure of chemical compounds and the chemical/physical properties (e.g., acid-base reactions, chemical kinetics) of these compounds.

Bodner and Domin (2000) and Coll and Treagust (2001) associated students' problem-solving ability with the type of mental models they construct. Bodner and Domin examined the number and types of representations constructed by both successful and unsuccessful problem solvers. They found that the successful problem solvers constructed more representations per problem than their counter cohort numbers constructed. Bodner and Domin also found that students who were not able to spontaneously switch from one representation to the other tended to perform poorly in organic chemistry. In contrast, students who did well in organic chemistry could switch back and forth between these representation systems as needed. Coll and Treagust indicated that experienced chemists tend to associate chemistry principles and chemical representations in a form of mental models. The mental models that chemists hold are abstract ideas, constructed based on the problem to solve, whereas undergraduate learners conceptualize more by word association. Findings of my analyses of students' conceptual frameworks and their reconciliation of different models provide a possible explanation for Bodner's and Domin's as well as Coll's and Treagust's observations.

Assertion 5. Advantages and difficulties of using concept webs to analyze student thinking. Concept web analysis in this study was an effective research tool to provide a visual aid to illustrate students' conceptual frameworks by showing the numbers of key concepts and connections, number of missing concepts and links, and misconceptions. The web structure provided a systematic way to examine the hierarchical structure of prerequisite and advanced concepts by analyzing the logic of students' explanations. Also, it allowed me to compare the similarities and differences among students' conceptual frameworks.

However, using this technique as a research tool was very time consuming. While developing nodes and links for each case and for within-case analyses, I encountered the following difficulties:

- It requires a researcher to interpret threads of thinking and students' meanings of the concepts by analyzing their verbal and nonverbal explanations and artifacts to illustrate those connections.
- It is difficult to capture students' use of terminology about a concept in the context of explanations and to reduce the bias of researcher's interpretations. For example, when a student describes that electron pairs in a molecule would want to stay as far apart from each other as possible so they can be "happy," this student may use the term as a metaphoric term or a teleological explanations. Thus, a researcher needs to interpret students' use of terminology carefully.
- Not all concept nodes would receive equal attention by a student. Therefore, there were some nodes that did not have enough information to identify whether it was accurate or inaccurate, or vague versus precise. A researcher cautiously must determine when to probe further and when to stop probing during the interview to gather enough information to judge the correctness of students' understanding. For

example, when KA described his understanding about chemical bonds, he said: "When I think of chemical bond, just think about if you have two atoms and there is a bond together, they would be covalent or ionic. Just whatever is holding the two things together." If the researcher stopped here, he or she may think that KA possessed a vague understanding about covalent bonding and ionic bonding. But when KA was probed further to explain why the two atoms would attract to each other, he said:

> The charges. Like the cations and anions. Opposites attract. I guess in that way, the charges, they have to be balanced. So like hydrogen is +1 and fluorine is -1 so those match up. The charges would be the same and they like to be together. (KA, interview)

KA's further explanations indicated that he had a misconception about ionic bonding. Therefore, the node of "ionic bond" in KA's concept web was illustrated as a misconception. When there are many prerequisite concepts to investigate in a conceptual framework, probing consistently to gather enough information for each concept and managing the length of interview within a limited amount of time becomes a dilemma for the researcher.

- While analyzing students' explanations, sometimes the connections among prerequisite concepts were implicit due to their use of language. It was hard to determine whether the link between two concepts was a strong, weak, missing, or incorrect connection, especially when analyzing explanations for low content knowledge students.
- When students responded to different problems associated with the same concept, such as determining polarity of a H_2S and a BF_3 molecule, students utilized different

strategies, logics, or justifications. Therefore, it was difficult to assign the connections among concepts.

Assertions about Students' Thinking with Mental Models – Interactions between Content Knowledge and Mental-Modeling Ability

Assertion 1. There is a positive interdependent relationship between an individual's level of content knowledge and mental-modeling ability. Based on the literature review, I approached this study thinking that there are two major learning impediments: (1) failure to construct and use mental models as tools of thinking and (2) fragmented conceptual framework that have major influences on students' conceptualization of molecular polarity. Thus, I expected to see some students who possessed sufficient understanding about chemistry principles but suffered from their low visualization skills to construct mental models. Also, I expected that some students could visualize and manipulate a 3D imaginary structure easily, yet were held back in their course performance due to not understanding the prerequisite concepts.

One major finding of this study is the positive interdependent relationship between level of content knowledge and mental-modeling ability. The trend in Table 24 shows a positive independent relationship between an individual's level of content knowledge and mental-modeling ability, where one may facilitate or hinder the other. Among the eight participants, no student was identified as possessing high content knowledge and low mental-modeling ability, or vice versa. However, content knowledge and mental-modeling ability, either independently or together, may influence an individual's ability to solve problems about molecular geometry and polarity. This finding aligned with Bodner's and Guay's (1997) descriptions regarding the correlation between student's spatial ability and their performance on highly spatial topics in chemistry. However, one thing needs to be mentioned that objects used in the Purdue Visualization of Rotations Test (ROT) involved only spatial information rather than chemistry content. Mental-modeling ability discussed in this study incorporated effects of participants' existing knowledge. Thus, the positive interdependent relationship between mental-modeling ability and content knowledge was more expectable.

When an individual constructs a mental model and uses it to make an inference, his or her mental-modeling ability and level of content knowledge interact as a dynamic process and should not be considered as two separate sets of characteristics. Table 24 shows how students in the HMMA group, such as JS and RE, possessed more complete and coherent conceptual frameworks. The analyses of JS's and RE's mental models (Table 23) showed that their conceptual frameworks provided information to construct a mental model that contained correct features and supplemented appropriate propositions to reason using the causal/dynamic mechanisms of the mental models. In addition, using metacognition, they identified the context of a problem, examined their quality of understanding, formed a mental model with correct spatial information, and chose appropriate propositions to apply to and manipulate their mental model. Meanwhile, they monitored the entire mental-modeling process and self-checked their mental models and answers.

The analyses showed that construction of a mental model with correct static features and spatial information is supported by accurate conceptions in the conceptual frameworks. Misconceptions and personal theories lead to the construction of a mental model with incorrect features and/or spatial information, and the resulting mental model eventually provides erroneous feedback and reinforces the misconception. For example, I described that SD misinterpreted the hybridization of atomic orbitals and generated a mental model of "personal space bubble" for the arrangement of electron pairs in an H_2S molecule. In SD's mind, this mental image seemed to fulfill the propositions about the VSEPR model as she understood them and helped her explain the polarity of H_2S successfully. Thus, she was satisfied with the planar mental model and rejected the concept that the arrangement of electron pairs should have a tetrahedral shape.

In addition, the formation of a mental model also plays a critical role in conceptualizing chemistry properties and principles. For example, visualizing a probability region of electron distribution supported the understanding of quantum mechanics descriptions. Also, visualizing a geometric structure in 3D and inspecting the model against the VSEPR model were found to be critical to students' comprehension of the spatial information regarding the electron pairs' farthest position in 3D.

Therefore, I propose that the relationship between the level of content knowledge and mental-modeling ability in an individual's mind is interdependent. Low mental-modeling ability hinders students from comprehending chemistry principles and from developing a coherent conceptual framework. Low level content knowledge and fragmented conceptual frameworks do not enable students to supply propositions for appropriate features and mechanisms of a mental model that they need to operate at higher levels mental-modeling.

Assertion 2. Students across all level had difficulties visualizing the tetrahedral arrangement and bond angle of an H_2S *molecule*. Analyses of participants' mental models indicated that 6 of the 8 participants did not visualize the arrangement of electron pairs for a bent molecule as a tetrahedral shape (e.g., H_2S). Additionally, understanding the 109.5° bond angle mathematically for a tetrahedral structure, was a common difficulty shared across different levels of content knowledge. Reasons for students' failure to visualize the tetrahedral shape and the bond angle were found to be different for high content knowledge students (e.g., RE and CR) than for moderate and low content knowledge students (e.g., SD, TA, KA, and JT).

For high content knowledge students their difficulty may have been due to not having an opportunity to reconcile the concepts about bond angles and the VSEPR model for the same molecule with and without lone pairs. Consider RE's explanation for her lack of recognition about the arrangement of electron pairs for H_2S:

> Part of the reason probably why I put them here [in a planar shape] is because up until this chemistry class, I've learned about the shapes of molecules, but I hadn't really…we only did the molecular geometry, like, this is a bent molecule. We did not say the shape of the electron [arrangement of electron pairs]…where the electrons are, we never did the shape of that. So I guess that's probably why I would not have put them here [in a tetrahedral shape] because I never thought about saying, okay, this is a bent molecule, but the shape of where the electrons are is tetrahedral. It was not a hard concept for me to get. It was just newer. I had two years of chemistry in high school, and I never thought about that. So it is something that I have not really thought about as much. [13:22-14:57] (RE, interview)

Possessing an understanding of the VSEPR model and comprehending the tetrahedral molecule with four identical bonds, the high content knowledge students were able to reconcile this new spatial information with their existing knowledge. They did so by examining the tetrahedral structure of electron pairs for H_2S against their existing mental model, such as a CCl_4 molecule, and the VSEPR model. However, students with lower content knowledge and mental-modeling ability experienced difficulties bridging these gaps; it appeared that they neither possessed appropriate propositions about the lone pairs and the VSEPR model, nor did they comprehend the tetrahedral structure in 3D.

Discussion

Based on the findings from the quantitative and qualitative phases of this study, students' scores on the diagnostic instruments EN, CB, and GP showed a reasonable power of prediction and reflected the results of interviews on the eight participants' level of understanding about concepts of molecular geometry, polarity, and prerequisite concepts. Taking advantage of the mixed-method design, the next question to ask is: Among the large student sample, how many students have learned concepts of molecular polarity successfully and how many students are still struggling with these concepts? Using the same criteria for categorizing the eight interview participants, I categorized students who completed at least two out of the three diagnostic instruments (n = 133) in the quantitative phase into low-, moderate-, high-, and mixed-scoring groups. Mixed-scoring defines students who received a low score on one instrument, and moderate and high scores on the other two instruments, respectively. These students could not be classified into the low-, moderate-, or high-scoring groups. Table 27 shows that only 15% of the students achieved a high level of understanding, and about 28% of the moderate-scoring students and 43% low-scoring students were struggling with concepts of molecular geometry and polarity.

The results of the current study suggest that at least two-thirds of the students leave the classroom with insufficient understanding about molecular geometry, polarity, and prerequisite concepts. Unless students' learning impediments indicated in this study are

Table 27

Categorization of Student Samples Based on their Scores on Instruments EN, CN, and GP

	Frequency	Percentage (n = 133)
High-scoring	20	15.0%
Moderate-scoring	38	28.6%
Low-scoring	57	42.9%
Mixed-scoring	18	13.5%

addressed, the moderate- and low-scoring students will encounter difficulties in future chemistry classes.

Implications

Implications for Teaching Chemistry

The quantitative phase of the study identified numerous students' misconceptions associated with molecular geometry, polarity, and prerequisite concepts. In addition, based on the comparison of conceptual frameworks across high, moderate, and low content knowledge groups, three key concept areas were identified including a) the concept of atomic structure, b) the concept of effective core charge and principles of electrostatic force, and c) quantum mechanics descriptions that need to be addressed for developing higher quality of conceptual frameworks when learning about molecular geometry and polarity. These findings provide college chemistry instructors and curriculum developers information about how these concepts associate with each other in students' conceptual frameworks and the prerequisite concepts. A chemistry instructor should plan the sequence of instruction to address the prerequisite concepts in order to facilitate the development of conceptual frameworks. Also, it is important to assess whether students' have learned the prerequisite concepts before moving on to the next level.

My analyses of students' mental-modeling ability showed that students could adopt visualization skills, such as rotating a molecular structure and examining the molecule from different angles, from using simulation software in laboratory. Wu, Krajcik, and Soloway (2001) suggested that students need to recognize the visual similarities and differences between 2D and 3D models through rotating and comparing these representations. To improve students' visualization skills, MMMA and LMMA students may need more opportunities than currently available to use a computer-based visualization tool to facilitate the development of visualization skills.

Analyses of students' mental models showed that students across high-, moderate-, and low-scoring groups had difficulties in visualizing the tetrahedral arrangement of electron pairs for H_2S and its bond angle. To address this difficulty in the chemistry classroom, an investigator may need different approaches for high-scoring students versus moderate- and low-scoring students. High-scoring students have sufficient understanding about prerequisite concepts and high mental-modeling ability. Thus providing opportunities for high-scoring students to examine different 3D geometric structures with the VSEPR model and to inspect the spatial information of these 3D structures carefully may be helpful to resolve this difficulty.

Constructing a mental model of a tetrahedral structure and applying a proposition to manipulate the model mentally may be challenging for moderate- and low-scoring students. Based on these findings, I recommend that chemistry instructors: a) provide opportunities to construct a 3D concrete model for different geometric structures, b) make connections between descriptive propositions of a theoretical model (e.g. the hybridization of atomic orbital for a H_2S molecule, bond angle) and the concrete model explicit, and c) facilitate the comprehension for how the VSEPR model is enacted on a model and to determine the molecular geometry and arrangement of electron pairs in three dimension using the concrete model. In addition, students' missing concepts, missing linkages, and misconceptions need to be remediated in addition to the improvement of mental-modeling ability.

To improve students' metacognition during the mental-modeling process, instructors should provide opportunities for students to inspect a concrete model against propositions and use an alternative approach to examine the model. Also, asking students to construct concrete models to represent chemistry concepts or explain a phenomenon, such as chemical bonding, and then evaluate the advantages and limitations of the model will help students to understand that each model has its own explanatory power and limitations.

Future Research

Based on findings and discussions of this study, I suggest following directions for future research on students' understanding about molecular polarity and their thinking process at the submicroscopic-symbolic domain:

1. The analyses of students' conceptual frameworks confirmed that when studying student learning about an advanced concept, the scope of the research needs to go beyond examining student understanding about a single concept to be studied. To study advanced or more abstract concepts, research on student learning should investigate conceptual frameworks including prerequisite concepts and the

hierarchical relationship among them. Using concept webs to analyze students' conceptual frameworks provides visual illustrations of missing concepts, missing linkages, and misconceptions in students' conceptual framework. However, using this technique as a tool for analyzing student understanding is very time consuming. Administration of diagnostic instruments permits a researcher to identify misconceptions for the prerequisite concepts; yet, the diagnostic items fail to reveal missing links among concepts (Griffard & Wandersee, 2001). Future research should investigate additional research methods to assess the hierarchical relationships among prerequisite and advanced conceptions in students' conceptual frameworks.

2. Research on students' mental-modeling processes and model-based reasoning needs to go beyond interpreting verbal explanations and start to include students' drawings, constructed artifacts (e.g., concrete models), and hand gestures. Interpreting students' explanations with their constructed models and hand gestures may reduce the chance of misinterpreting students' use of language and the level of understanding. For example, when AM explained the repulsion between lone pairs and bonding pairs of H_2S based on a 2D Lewis structure, she described the repulsion between each electron pair as if they were on the same plane. But when she used a concrete model to show the spatial information of the molecule, she constructed a tetrahedral structure and successfully used it to solve a problem. AM's understanding about molecular geometry would be underestimated if a researcher merely used her drawings to interpret her explanations. The findings of this study echo Givry's and Roth's (2006) call that future research needs to reconceptualize the notion of conception to include

not only talk and gesture, but also the context during the interview, as dialectical units during a participant's meaning-making process.

3. The analysis of mental-modeling ability in this study is a first attempt to explore the mental-modeling process. In this study, a protocol comprising four characteristics associated with visualization skills and metacognition was developed. However, the protocol is not an exhaustive list. In order to understand the mental-modeling process and to identify the actions that are critical for successful learning and problem-solving, more research needs to be devoted to developing a typology of mental-modeling actions.
4. I also found that metacognitive ability plays a significant role in a successful mental-modeling. Various conceptual change theories (Hewson, 1981; She, 2004; Tyson, Venville, Harrison, & Treagust, 1997; Vosniadou, 2003; Vosniadou & Ioannides, 1998) have included metacognition as a crucial aspect when studying conceptual change processes. However, metacognition has not been discussed in research on students' mental models or model-based reasoning. Therefore, future research agenda should include an exploration on the role of metacognition in the mental-modeling process.
5. A major finding of this research is the positive interdependent relationship between an individual's level of content knowledge and mental-modeling ability. During the interviews, I observed that students' thinking process with mental models was a dynamic process where multiple interactions between applying propositions to the model and mental-modeling ability occurring in seconds. Future research needs to closely examine the mental-modeling process in action in order to provide

explanations for how content knowledge and mental-modeling ability enhance or hinder each other.

6. The analyses of conceptual frameworks also indicated students' level of content knowledge was related to the quality of their explanations. High content knowledge students could justify their answers and explanations with other correct concepts or propositions. When the quality of conceptual frameworks decreases and knowledge became fragmented, students used algorithmic strategies, developed personal theories, or utilized teleological or anthropomorphic explanations to explain their answers. Future research should explore the relationship between students' quality of conceptual frameworks and quality of explanations from an epistemological perspective; and also, how the quality of conceptual frameworks influences their reasoning patterns.

Research has shown that molecular polarity is a difficult concept for students to understand (Furió & Calatayud, 1996; Furió et al., 2000; Peterson et al., 1989); yet, literature focused on student understanding of molecular polarity is limited (Furió & Calatayud, 1996). Previous studies in the submicroscopic-symbolic domain have focused on one of the three aspects including students' content knowledge, features of mental models about a specific concept, and visual-spatial thinking ability. This study fills a void by examining these three aspects together to find out how these aspects interact and influence students' understanding about concepts of molecular geometry and polarity. In this study, I found a positive interdependent relationship between an individual's level of content knowledge and mental-modeling ability. This study also provides evidence showing that when a student constructs a mental model to solve a problem, both of his or her content knowledge and mental-modeling ability may facilitate one or hinder another.

In terms of the research design, previous research on molecular polarity used a quantitative phase to describe students' understanding (Furió & Calatayud, 1996; Furió et al., 2000; Jang, 2003; Peterson et al., 1989). Briggs (2004) and Stieff et al. (2005) called for a new perspective to focus on the nature and process of the thinking mind, a perspective that accounts for the role of visualization and comprehension. To respond to their call, I developed thought-eliciting tasks and used video-taping to capture students' visualization, comprehension, and thinking process for their verbal explanations, constructions of artifacts, and hand gestures. I learned that thinking with models and/or mental models is a rich and dynamic process. Merely analyzing students' responses to diagnostic test items, verbal explanations, and drawings will omit important information and lead to misinterpretations of students' understanding. Moreover, the quantitative phase of this study allowed me to collect information about student understanding and misconceptions for the targeted concept and its prerequisite conceptions on a large student number. The quantitative data also supported a purposeful sampling at the qualitative phase of the study as well as the data triangulation between quantitative and qualitative findings. The purposeful sampling and data triangulation permitted the generalization of qualitative findings to a greater number of students. This study demonstrated that, by using a mixed-method design, research on student thinking can incorporate the strengths of quantitative and qualitative research.

REFERENCES

Ardac, D., & Akaygum, S. (2004). Effectiveness of multimedia-based instruction that emphasizes molecular representations on students' understanding of chemical change. *Journal of Research in Science Teaching, 41*, 317-337.

Ben-Zvi, R., Eylon, B.-S., & Silberstein, J. (1987). Students' visualization of a chemical reaction. *Education in Chemistry, July*, 117-120.

Bodner, G. M., & Domin, D. S. (2000). Mental models: The role of representations in problem solving in chemistry. *University Chemistry Education, 4*(1), 24-30.

Bodner, G. M., & Guay, R. B. (1997). The Purdue Visualization of Rotations Test. *The Chemical Educator, 2*(4), 1-17.

Borges, A. T., & Gilbert, J. K. (1999). Mental models of electricity. *International Journal of Science Education, 21*, 95-117.

Bransford, J. D., Brown, A. L., & Cocking, R. R. (1999). *How people learn: Brain, mind, experience, and school*. Washington, D.C.: National Academies Press.

Briggs, M. W. (2004). *A cognitive model of second-year organic students' conceptualizations of mental model rotation.* Unpublished doctoral dissertation, Purdue University.

Briggs, M. W. (2007). Models and modeling. In M. Orgill & G. M. Bodner (Eds.), *Theoretical frameworks for research in chemistry/science education* (pp. 69-83). Upper Saddle River, NJ: Prentice Hall.

Briggs, M. W., & Bodner, G. M. (2005). A model of molecular visualization. In J. K. Gilbert (Ed.), *Visualization in science education* (pp. 61-73). Netherlands: Springer.

Buckley, B. C., & Boulter, C., J. (2000). Investigating the role of representations and expressed model in building mental models. In J. K. Gilbert & C. J. Boulter (Eds.), *Developing models in science education* (pp. 119-135). Netherlands: Kluwer Academic Publishers.

Chang, R. (2005). *Chemistry* (8th ed.). New York: McGraw-Hill.

Chi, M. T. H. (1992). Conceptual change within and across ontological categories: Examples from learning and discovery in science. In R. Giere (Ed.), *Cognitive models of science: Minnesota studies in the philosophy of science* (pp. 129-160). Minneapolis, MN: University of Minnesota Press.

Chi, M. T. H., Slotta, J. D., & de Leeuw, N. (1994). From things to processes: A theory of conceptual change for learning science concepts. *Learning and Instruction, 4*, 27-43.

Chiu, M.-H. (2007). A national survey of students' conceptions of chemistry in Taiwan. *International Journal of Science Education, 29*, 421-452.

Chiu, M.-H., Chou, C.-C., & Liu, C.-J. (2002). Dynamic processes of conceptual change: Analysis of constructing mental models of chemical equilibrium. *Journal of Research in Science Teaching, 39*, 688-712.

Cokelez, A., & Dumon, A. (2005). Atom and molecule: Upper secondary school French students' representations in long-term memory. *Chemical Education: Research and Practice, 6*, 119-135.

Coll, R. K., & Taylor, N. (2001). Alternative conceptions of chemical bonding held by upper secondary and tertiary students. *Research in Science and Technological Education, 19*, 171-191.

Coll, R. K., & Treagust, D. F. (2001). Learners' mental models of chemical bonding. *Research in Science Education, 31*, 357-382.

Coll, R. K., & Treagust, D. F. (2002). Exploring tertiary students' understanding of covalent bonding. *Research in Science and Technological Education, 20*, 241-267.

Coll, R. K., & Treagust, D. F. (2003a). Investigation of secondary school, undergraduate, and graduate learners' mental models of ionic bonding. *Journal of Research in Science Teaching, 40*, 464-486.

Coll, R. K., & Treagust, D. F. (2003b). Learners' mental models of metallic bonding: A cross-age study. *Science Education, 87*, 685-707.

Donovan, M. S., & Bransford, J. D. (2005). *How students learn science in the classroom*. Washington, D.C.: National Academies Press.

Driver, R., Squires, A., Rushworth, P., & Wood-Robinson, V. (1994). *Making sense of secondary science: Research into children's ideas*. New York: RoutledgeFalmer.

Eilam, B. (2004). Drops of water and soap solution: Students' constraining mental models of the nature of matter. *Journal of Research in Science Teaching, 41*, 970-993.

Ferguson, R. L. (2007). Constructivism and social constructivism. In M. Orgill & G. M. Bodner (Eds.), *Theoretical frameworks for research in chemistry/science education* (pp. 27-48). Upper Saddle River, NJ: Prentice Hall.

Ferk, V., Vrtacnik, M., Blejec, A., & Gril, A. (2003). Students' understanding of molecular structure representations. *International Journal of Science Education, 25*, 1227-1245.

Franco, C., & Colinvaux, D. (2000). Grasping mental model. In J. K. Gilbert & C. J. Boulter (Eds.), *Developing models in science education* (pp. 93-117). Netherlands: Kluwer Academic Publishers.

Furió, C., & Calatayud, M. L. (1996). Difficulties with the geometry and polarity of molecules. *Journal of Chemical Education, 73*, 36-41.

Furió, C., Calatayud, M. L., Bárcenas, S. L., & Padilla, O. M. (2000). Functional fixedness and functional reduction as common sense reasonings in chemical equilibrium and in geometry and polarity of molecules. *Science Education, 84*, 545-565.

Gabel, D. (1998). The complexity of chemistry and implications for teaching. In B. J. Fraser & K. G. Tobin (Eds.), *International handbook of science education* (pp. 233-248). Netherlands: Kluwer Academic Publishers.

Givry, D., & Roth, W.-M. (2006). Toward a new conception of conceptions: Interplay of talk, gestures, and structures in the setting. *Journal of Research in Science Teaching, 43*, 1086-1109.

Glynn, S. M., & Duit, R. (1995). Learning science meaningfully: Constructing conceptual model. In S. M. Glynn & R. Duit (Eds.), *Learning science in the schools: Research reforming practice* (pp. 3-33). Mahwah, NJ: Lawrence Erlbaum Associates.

Greca, I. M., & Moreira, M. A. (2000). Mental models, conceptual models, and modelling. *International Journal of Science Education, 22*, 1-11.

Griffard, P. B., & Wandersee, J. H. (2001). The two-tier instrument on photosynthesis: What does it diagnose? *International Journal of Science Education, 23*, 1039-1052.

Grosslight, L., Unger, C., & Jay, E. (1991). Understanding models and their use in science: Conceptions of middle and high school students and experts. *Journal of Research in Science Teaching, 28*, 799-822.

Harrison, A. G., & Treagust, D. F. (1996). Secondary students' mental models of atoms and molecules: implications for teaching chemistry. *Science Education, 80*, 509-534.

Harrison, A. G., & Treagust, D. F. (2000). Learning about atoms, molecules, and chemical bonds: a case study of multiple-model use in Grade 11 chemistry. *Science Education, 84*, 352-381.

Hewson, P. W. (1981). A conceptual change approach to learning science. *European Journal of Science Education, 3*, 383-396.

Hewson, P. W. (1996). Teaching for conceptual change. In D. F. Treagust, R. Duit & B. J. Fraser (Eds.), *Improving teaching & learning in science and mathematics* (pp. 131-140). NY: Cambridge University Press.

Hewson, P. W., & Hewson, M. G. (1992). The status of students' conceptions. In R. Duit, F. Goldberg & H. Niedderer (Eds.), *Research in physics learning: Theoretical issues and empirical studies. Proceedings of an international workshop hold at the University of Bremen, March, 1991* (pp. 203-224): Kiel: IPN.

Hinton, M. E., & Nakhleh, M. B. (1999). Students' microscopic, macroscopic, and symbolic representations of chemical reactions. *Chemical Educator, 4*, 158-167.

Jang, N. H. (2003). *Developing and validating a chemical bonding instrument for Korean high school students.* Unpublished doctoral dissertation, University of Missouri-Columbia.

Johnstone, A. H. (1991). Why is science difficult to learn? Things are seldom what they seem. *Journal of Computer Assisted Learning, 7*, 75-83.

Johnstone, A. H. (1993). The development of chemistry teaching: A changing response to changing demand. *Journal of Chemical Education, 70*, 701-705.

Kleinman, R. W., Griffin, H. C., & Kerner, N. K. (1987). Images in chemistry. *Journal of Chemical Education, 64*, 766-770.

Kousathana, M., & Tsaparlis, G. (2002). Students' errors in solving numerical chemical-equilibrium problems. *Chemical Education: Research and Practice in Europe, 3*, 5-17.

Krajcik, J. S. (1991). Developing students' understanding of chemical concepts. In S. M. Glynn, R. H. Yeany & B. K. Brutton (Eds.), *The psychology of learning science* (pp. 117-147). Hillsdale, NJ: Lawrence Erlbaum Associates.

Lee, K.-W. L. (1999). A comparison of university lectures' and pre-service teachers' understanding of a chemical reaction at the particulate level. *Journal of Chemical Education, 76*, 1008-1012.

Lichtfeldt, M. (1996). Development of pupils' ideas of the particulate nature of matter: long-term research project. In G. Welford, J. Osorne & P. Scott (Eds.), *Research in science education in Europe: Current issues and themes* (pp. 212-228). Washington D.C.: The Falmer Press.

Lincoln, Y. S., & Guba, E. G. (1985). *Naturalistic inquiry*. Thousand Oaks, CA: Sage Publications, Inc.

Marais, P., & Jordaan, F. (2000). Are we taking symbolic language for granted? *Journal of Chemical Education, 77*, 1355-1357.

Mathewson, J. H. (1999). Visual-spatial thinking: An aspect of science overlooked by educators. *Science Education, 83*, 33-54.

Mortimer, E. F. (1995). Conceptual change or conceptual profile change? *Science & Education, 4*, 267-285.

Mulford, D. R., & Robinson, W. R. (2002). An inventory for a alternate conceptions among first-semester general chemistry students. *Journal of Chemical Education, 79*, 739-744.

Nicoll, G. (2001). A report of undergraduates' bonding misconceptions. *International Journal of Science Education, 23*, 707-730.

Nicoll, G. (2003). A qualitative investigation of undergraduate chemistry students' macroscopic interpretations of the submicroscopic structure of molecules. *Journal of Chemical Education, 80*, 205-213.

O'Connor, E. A. (1997). *Atomic and molecular models in learning chemistry.* Unpublished doctoral dissertation, University at albany, State University of New York, Albany, New York.

Ophardt, C. (2003). Molecular polarity. *Virtual chembook* Retrieved February 3, 2007, from http://www.elmhurst.edu/~chm/vchembook/210polarity.html

Patton, M. Q. (2002). *Qualitative research and evaluation methods* (3rd ed.). Thousand Oaks, CA: Sage Publications, Inc.

Peterson, R. F., & Treagust, D. F. (1989). Grade-12 students' misconceptions of covalent bonding and structure *Journal of Chemical Education, 66*, 459-460.

Peterson, R. F., Treagust, D. F., & Garnett, P. (1989). Development and application of a diagnostic instrument to evaluate grade-11 and -12 students' conceptions of covalent bonding and structure following a course of instruction. *Journal of Research in Science Teaching, 26*, 301-314.

Posner, G. J., Strike, K. A., Hewson, P. W., & Gertzog, W. A. (1982). Accommodation of a scientific conception: Toward a theory of conceptual change. *Science Education, 66*, 211-227.

Ringnes, V. (1994). Students' understanding of chemistry and their learning difficulties. In H.-J. Schmidt (Ed.), *Proceedings of the 1994 international symposium: Problem solving and misconceptions in chemistry and physics* (pp. 100-112). Dortmund, Germany: The International Council of Association for Science Education.

Roth, W.-M., Pozzer-Ardenghi, L., & Han, J. Y. (2005). Semiotics of chemical inscriptions. In *Critical graphicacy: Understanding visual representation practices in school science* (Vol. 26, pp. 187-216). Netherlands: Springer.

Scott, P. H. (1992). Pathways in learning science: A case study of the development of one student's ideas relating to the structure of matter. In R. Duit, F. Goldberg & H. Niedderer (Eds.), *Research in physics learning: Theoretical issues and empirical studies. Proceedings of an international workshop hold at the University of Bremen, March, 1991* (pp. 203-224). Kiel: IPN.

Seddon, G. M., Eniaiyejy, P. A., & Chia, L. H. L. (1985). The factor structure for mental rotations of three-dimensional structures represented in diagrams. *Research in Science and Technological Education, 4*, 29-37.

Shane, J. W., & Bodner, G. M. (2006). General chemistry students' understanding of structure-function relationships. *Chemical Educator, 11*, 130-137.

She, H.-C. (2002). Concepts of a higher hierarchical level require more dual situated learning events for conceptual change: a study of air pressure and buoyancy. *International Journal of Science Education, 24*, 981-996.

She, H.-C. (2004). Fostering radical conceptual change through dual-situated learning model. *Journal of Research in Science Teaching, 41*, 142-164.

Stieff, M., Bateman, R., & Uttal, D. (2005). Teaching and learning with three-dimensional representations. In J. K. Gilbert (Ed.), *Visualization in science education* (pp. 93-121). Netherlands: Springer.

Strauss, A., & Corbin, J. (1998). *Basic of qualitative research: Techniques and procedures for developing grounded theory*. Thousand Oaks, CA: Sage Publications, Inc.

Strike, K. A., & Posner, G. J. (1992). A revisionist theory of conceptual change. In R. A. Duschl & R. J. Hamilton (Eds.), *Philosophy of science, cognitive psychology, and educational theory and practice* (pp. 147-176). Albany, NY: State University of New York Press.

Taber, K. S. (2000). Case studies and generalizability: Grounded theory and research in science education. *International Journal of Science Education, 22*, 469-487.

Taber, K. S. (2001a). Building the structural concepts of chemistry: Some considerations from educational research. *Chemistry Education: Research and Practice in Europe, 2*, 123-158.

Taber, K. S. (2001b). Shifting sands: a case study of conceptual development as competition between alternative conceptions. *International Journal of Science Education, 23*, 731-753.

Taber, K. S. (2002a). *Chemical misconception - Prevention, diagnosis and cure: Volume I: Theoretical background*. London: Royal Society of Chemistry.

Taber, K. S. (2002b). *Chemical misconception - Prevention, diagnosis and cure: Volume II: Classroom resources*. London: Royal Society of Chemistry.

Taber, K. S. (2003a). Mediating mental models of materials: Acknowledging the priority of the learner's prior learning. *Science Education, 87*, 732-758.

Taber, K. S. (2003b). Understanding ionisation energy: Physical, chemical, and alternative conceptions. *Chemical Education: Research and Practice in Europe, 4*, 149-169.

Talanquer, V. (2006). Commonsense chemistry: A model for understanding student's alternative conceptions. *Journal of Chemical Education, 83*, 811-816.

Talanquer, V. (in press). Explanations and teleology in chemistry education. *International Journal of Science Education*.

Tan, K.-C., & Treagust, D. F. (1999). Evaluating students' understanding of chemical bonding. *School Science Review, 81*, 75-83.

Treagust, D. F. (1995). Diagnostic assessment of students' science knowledge. In S. M. Glynn & R. Duit (Eds.), *Learning science in the schools: Research reforming practice*. Mahwah, NJ: Lawrence Erlbaum Associates.

Treagust, D. F., & Chandrasegaran, A. L. (2007). The Taiwan national science concept learning study in an international perspective. *International Journal of Science Education, 29*, 391-403.

Treagust, D. F., & Chittleborough, G. (2001). Chemistry: A matter of understanding representations. In J. Brophy (Ed.), *Subject-Specific Instructional Methods and Activities* (Vol. 8, pp. 239-267). Oxford, UK: Elsevier Science Ltd.

Tuckey, H., Selvaratnam, M., & Bradley, J. (1991). Identification and rectification of student difficulties concerning three-dimensional structures, rotation, and reflection. *Journal of Chemical Education, 68*(460-464).

Tyson, L. M., Venville, G. J., Harrison, A. G., & Treagust, D. F. (1997). A multidimensional framework for interpreting conceptual change events in the classroom. *Science Education, 81*, 387-404.

Undergraduate 2006-2008 Catalog Extracts: College of Art and Science. (2006). Retrieved September 18, 2006, from http://registrar.missouri.edu/Catalog/extracts_06_08/A&S.pdf

Vogt, W. P. (2007). *Quantitative research methods for professionals*. Boston: Pearson Education.

Vosniadou, S. (1994). Capturing and modeling the process of conceptual change. *Learning and Instruction, 4*, 45-69.

Vosniadou, S. (2003). Exploring the relationships between conceptual change and intentional learning. In G. M. Sinatra & P. R. Printrich (Eds.), *Intentional conceptual change* (pp. 377-406). Mahwah, NJ: Lawrence Erlbaum Associates.

Vosniadou, S., & Brewer, W. (1992). Mental models of the Earth: A study of conceptual change in childhood. *Cognitive Psychology, 24*, 535-585.

Vosniadou, S., & Ioannides, C. (1998). From conceptual development to science education: A psychological point of view. *International Journal of Science Education, 20*, 1213-1230.

White, R. T., & Gunstone, R. F. (1992). *Probing understanding*. New York: The Falmer Press.

Williamson, V. M., & Abraham, M. R. (1995). The effects of computer animation on the particulate mental models of college chemistry students. *Journal of Research in Science Teaching, 32*, 521-534.

Wu, H.-K., Krajcik, J. S., & Soloway, J. S. (2001). Promoting understanding of chemical representations: Students' use of a visualization tool in the classroom. *Journal of Research in Science Teaching, 38*, 821-842.

Wu, H.-K., & Shah, P. (2004). Exploring visuospatial thinking in chemistry learning. *Science Education, 88*, 465-492.

Zohar, A., & Ginossar, S. (1998). Lifting the taboo regarding teleology and anthropomorphism in biology education—Heretical Suggestions. *Science Education, 82*, 679-697.

APPENDIX A

CONSENT FORM

CONSENT FORM

November ___, 2006
Dear Chemistry 1320 Student,

I am a doctoral student in science education at the University of Missouri-Columbia (MU) conducting my dissertation research on college students' learning about molecular polarity. The study is taking place in this Chemistry 1320 class during the Fall 2006 semester.

Science educators, like myself, have focused upon what to teach and how to teach it. However, not much is known about what's going on in students' mind when they try to make sense of a new chemical concept. I believe that learning is more than just sit and listen. Professors can teach better if they know what and how to do to help students understand, but we need your assistance in helping us determine what's effective for the student.

Molecular polarity is a foundation for learning concepts like intermolecular forces, solutions, acids and bases, and organic chemistry. It is also known as an abstract concept that requires students to think in three dimensions. Learning a concept like this requires more than reading the textbook and listening to the lecture. I believe that it is something in a person's thinking process that makes his/her learning different. I hope you will be interested in contributing to this understanding of why molecular polarity is difficult for some students to understand. I'm asking for volunteers to provide me with your insights into what comes to your mind and how you solve it while working through general chemistry problems.

Your participation is totally optional. The professor will not know who is or is not participating. However, if you are willing to participate, you can choose to do so at one of three levels:

	Type of Study Participation	Your Time Commitment
1	Provide access to your answers on (1) any homework assignment and course examine, and (2) your information about ACT score, SAT score, and the number of chemistry course you took at high school and university prior to this course.	NONE!
2	Provide access to your answers on (1) any homework assignment and course examine, and (2) your information about ACT score, SAT score, and the number of chemistry course you took at high school and university prior to this course, PLUS share with me your thinking process while working through general chemistry problems in an interview	1 hour 45 min interview during the semester

The problems used in the interview are aligned with this course. This interview may benefit you by refreshing and reorganizing concepts you have learned from the class. At the end of the interview, I will also share with you about the textbook explanations to these problems as a mini tutor section.

The study is being conducted to provide a better understanding of how students apply their knowledge and what mental image they have while thinking about general chemistry problems. The interview would be scheduled at a time and location convenient to you. If you agree, interviews will be audio and video taped to ensure accurate data collection and to facilitate my data analysis. Audio and video tapes will be kept on file for no more than three years.

You must be 18 years old to participate in this study and your participation is completely voluntary. If you agree to participate, you may choose not to answer any question. You may withdraw from the study at any time without consequences to you. Your confidentiality will be strictly protected. Your name will be replaced with a code. Only the researcher (Chia-Yu Wang) will have access to the master list that matches your name with the code. Audio and Video tapes from interviews will be transcribed by the student investigator or a university transcriptionist. As soon as the transcriptions are complete, all tapes will be securely stored.

NO results will be reported in a manner that would allow a reader to associate any responses to you. Confidentiality will also be kept if data are shared at professional presentations and in scholarly publications. Participating in the study will subject you to no risks greater than those you normally encounter in everyday life.

Please feel free to ask any question during or after your participation in this study. If you have questions or concerns about this study, you may contact me:

Chia-Yu Wang
321-L Townsend Hall
University of Missouri – Columbia
Columbia, MO 65211
e-mail cwg25@mizzou.edu
phone (573) 882-5485

For questions concerning human subjects research, you may contact the MU Campus Institutional Review Board at:

Campus IRB Compliance Office
483 McReynolds Hall
Columbia, MO 65211
(573) 882-9585

You also may email the Campus IRB Compliance Office at umcresearchcirb@missouri.edu.

Your signature on the adjoining consent form indicates that you have received a copy, read, and understand this letter that describes the study. An informed written consent is required by IRB for your participation.

Thank you so much!
Sincerely,

Chia-Yu Wang
PhD Candidate – Science Education

Lloyd H. Barrow
Professor Science Education
Dissertation Supervisor

Informed Consent Form

General Chemistry Students' Understanding about Molecular Polarity

Please indicate what your decision is regarding participation in this study by checking one box indicating your choice, signing and then dating the consent form.

☐ I AGREE TO PARTICIPATE in the 'General Chemistry Students' Understanding about Molecular Polarity' study being conducted by a graduate student investigator, Chia-Yu Wang, at the University of Missouri – Columbia. I understand that my participation is voluntary and that I may withdraw at any time without consequences to me. I know that my participation has no bearing upon my course grade.

Circle a number below to indicate your level of participation:

1 I agree to grant access to my answers on (1) any homework assignment and course exam, and (2) my information about the number of chemistry courses I took at high school and university prior to this course. I understand that there will be NO extra time commitment on my part.

2 I agree to grant access to my answers on (1) any homework assignment and course exam, (2) my information about the number of chemistry courses I took at high school and university prior to this course, and share my thinking process while working through general chemistry problems in a 1 hour interview to be scheduled at my convenience during the semester.

______________________________ __________________________
Signature Date

______________________________ __________________________
Name (Please Print) Student number

____
Email address

☐ I DECLINE TO PARTICIPATE in the 'General Chemistry Students' Understanding about Molecular Polarity' study being conducted by a graduate student investigator, Chia-Yu Wang, at the University of Missouri – Columbia. I know that my decision has no bearing upon my course grade.

______________________________ ______________________________
Signature Date

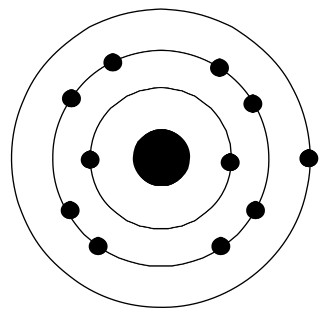
____
Name (Please Print)

APPENDIX B

INSTRUMENT EN

INSTRUMENT EN

The statements below refer to this diagram of the electronic structure of an atom. Please read each statement carefully, and decide whether it is correct or not.



1. Energy is required to remove an electron from the atom.
2. After the atom is ionised, it then requires more energy to remove a second electron because the second electron is nearer the nucleus.
3. The atom will spontaneously lose an electron to become stable.
4. Only one electron can be removed from the atom, as it then has a stable electronic configuration.
5. The nucleus is not attracted to the electrons.
6. Each proton in the nucleus attracts one electron.
7. After the atom is ionised, it then requires more energy to remove a second electron because the second electron experiences less shielding from the nucleus.
8. The nucleus is attracted towards the outermost electron less than it is attracted towards the other electrons.
9. After the atom is ionised, it then requires more energy to remove a second electron because the second electron is in a lower energy level.
10. After the atom is ionised, it then requires more energy to remove a second electron because it experiences a greater core charge than the first.
11. After the atom is ionised, it then requires more energy to remove a second electron because it would be removed from a positive species.
12. If the outermost electron is removed from the atom it will not return because there will be a stable electronic configuration.
13. The force on an innermost electron from the nucleus is equal to the force on the nucleus from an innermost electron.
14. Electrons do not fall into the nucleus as the force attracting the electrons towards the nucleus is balanced by the force repelling the nucleus from the electrons.

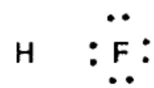
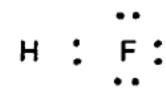
15. The third ionisation energy is greater than the second as there are less electrons in the shell to share the attraction from the nucleus.
16. The force pulling the outermost electron towards the nucleus is greater than the force pulling the nucleus towards the outermost electron.
17. After the atom is ionised, it then requires more energy to remove a second electron because once the first electron is removed the remaining electrons receive an extra share of the attraction from the nucleus.
18. The atom would be more stable if it ‘lost’ an electron.
19. The eleven protons in the nucleus give rise to a certain amount of attractive force that is available to be shared between the electrons.
20. The atom would become stable if it either lost one electron or gained seven electrons.

APPENDIX C

INSTRUMENT CB

INSTRUMENT CB

1. Which of the following best represents the position of the shared electron pair in the HF molecule

(1)  (2) 

<u>Reason</u>

(A) Non-bonding electrons influence the position of the bonding or shared electron pair.

(B) As hydrogen and fluorine form a covalent bond the electron pair must be shared equally.

(C) Fluorine has a stronger attraction than hydrogen for the shared electron pair.

(D) Fluorine is the larger of the two atoms and hence exerts greater control over the shared electron pair.

2. The polarity of the oxygen-fluorine bond is best shown as

(1) $\overset{\delta^-}{O}—\overset{\delta^+}{F}$ (2) $\overset{\delta^+}{O}—\overset{\delta^-}{F}$

<u>Reason</u>

(A) The non-bonding electron pairs present on each atom determine the polarity of the bond.

(B) A polar covalent bond forms because oxygen has six outer shell electrons and fluorine seven outer shell electrons.

(C) The shared electron pair is more closely associated with the fluorine atom.

(D) The polarity of the bond is due to the oxygen atom forming an O^{2-} ion, whereas fluorine forms as F^- ion.

3. Silicon carbide has a high melting point and a high boiling point.
This suggests silicon carbide has

(1) strong covalent bonds (2) strong intermolecular forces

<u>Reason</u>

(A) Silicon carbide is a covalent network solid (continuous covalent lattice) composed of covalently bonded molecules.

(B) A large amount of energy is required to break the intermolecular forces in the silicon carbide lattice.

(C) Silicon carbide is a covalent molecular solid.

(D) Silicon carbide is a covalent network solid (continuous covalent lattice) composed of covalently bonded atoms.

4. The most important particle of chemical bonding is:

(1) the proton in the outer shell.
(2) all electrons
(3) the electron in the outer shell

<u>Reason</u>

(A) The chemical bonding is due to the proton transfer.

(B) The chemical bonding is due to all electrons' transfer.

(C) The chemical bonding is due to all electrons' loss.

(D) The chemical bonding is due to the electron transfer in the outer shell.

5. The state of the electrons for an ionic bonding is:

(1) electron sharing (2) electron transfer (3) electron destroying

<u>Reason</u>

(A) Electrons of atoms will be shared with the same number of electrons.

(B) Electrons of atoms will be entirely transferred to other atom.

(C) Electrons of atoms will be entirely destroyed.

(D) Electrons of atoms will be entirely divided into other atom.

6. Sodium chloride, NaCl, exists as a molecule:

(1) True (2) False

<u>Reason</u>

(A) The sodium atom shares a pair of electrons with the chlorine atom to forms a simple molecule.

(B) After donating its valence electron to the chloride atom, the sodium ion forms a molecule with the chloride ion.

(C) Sodium chloride exists as a lattice consisting of sodium ions and chloride ions.

(D) Sodium chloride exists as a lattice consisting of covalently bonded sodium and chloride atoms.

7. The kind of bonding to make the water molecule (H_2O) is:

(1) ionic bonding
(2) polar covalent bonding
(3) non-polar covalent bonding

<u>Reason</u>

(A) Hydrogen loses an electron to be the hydrogen ion H^+.

(B) Oxygen gains two electrons to be the oxygen ion O^{2-}.

(C) Hydrogen and oxygen share electrons equally.

(D) The electronegativity of oxygen is larger than that of hydrogen.

APPENDIX D

INSTRUMENT GP

1. Nitrogen (a group 5 element) combines with bromine (a group 7 element) to form a molecule. This molecule is likely to have a shape which best described as
   (1) trigonal planar
   (2) trigonal pyramidal
   (3) tetrahedral

   Reason

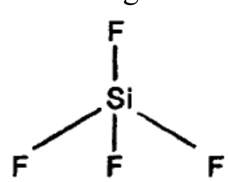
   (A) Nitrogen forms three bonds which equally repel each other to form a trigonal planar shape.

   (B) The tetrahedral arrangement of the bonding and non-bonding electron pairs around the nitrogen atom determines the shape of the molecule.

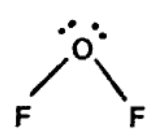
   (C) The polarity of each nitrogen-bromine bond determines the shape of the molecule.

   (D) The difference in the electronegativity values for bromine and nitrogen determines the shape of the molecule.

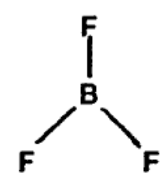
2. Which one of the following molecules is polar?



(1)



(2)



(3)

   Reason

   (A) The polarity of the molecule is due to the high electronegativity of fluorine.

   (B) Non-symmetrical molecules containing atoms of differing electronegativity are polar.

   (C) Non-bonding electrons on an atom in the molecule produce a dipole and hence a polar molecule.

   (D) A large difference in the electronegativities of the atoms involved in bonding results in a polar molecule.

3. The molecule SCl_2 is

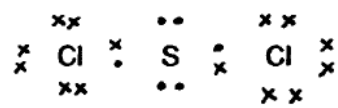
(1) v-shaped (2) linear

<u>Reason</u>

(A) Repulsion between the bonding and non-bonding electron pairs of the sulphur atom determines the shape.

(B) Repulsion between the non-bonding electron pairs determines the shape.

(C) The two sulfur-chlorine bonds are equally repelled to linear positions because SCl_2 has an electron dot structure shown as



(D) The high electronegativity of chlorine compared with sulfur is the major factor influencing the shape of the molecule.

4. Water (H_2O) and hydrogen sulfide (H_2S) have similar chemical formulae and have V-shaped structures. The difference in state between water (liquid) and hydrogen sulphide (gas) is due to

(1) strong intermolecular forces between H_2S molecules
(2) strong intermolecular forces between H_2O molecules
(3) weak intermolecular forces between H_2O molecules

<u>Reason</u>

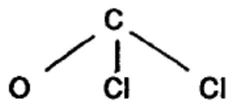
(A) The difference in strength of the intermolecular forces is due to the difference in strength of O-H and S-H covalent bonds.

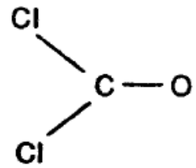
(B) The bonds in H_2S are easily broken, whereas in H_2O they are not.

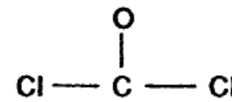
(C) The difference in strength of the intermolecular forces is due to the difference in polarity of the molecules

(D) The difference in strength of the intermolecular forces is due to the fact that H_2O is a polar molecule, where H_2S is a non-polar molecule.

5. Which of the following best indicates the shape of the $COCl_2$ molecule

(1) 

(2) 

(3) 

<u>Reason</u>

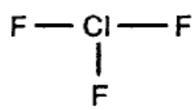
(A) The shape of the $COCl_2$ is dependent on the electronegativity of each atom.

(B) The shape of the $COCl_2$ is due to approximately equal repulsion between the bonding and non-bonding electron pairs on the carbon.

(C) The shape of the $COCl_2$ is due to the stronger polarity of the C=O double bond in the molecule

(D) The shape of the $COCl_2$ is due to equal repulsion between the bonding regions formed by the atoms joining to the carbon.

6. The substance chlorine trifluoride (ClF_3) is as a planar, T-shaped molecule. Its structure can be represented as



Based on this information ClF_3 is most likely to be a

(1) polar molecule (2) non-polar molecule

<u>Reason</u>

(A) The molecule is polar because it has polar bonds.

(B) As fluorine has a very high electronegativity the molecule is polar.

(C) The T-shaped arrangement of the polar bonds results in a polar molecule.

(D) The molecule is non-polar because there is very little difference between the electronegativities of Cl and F.

7. The octet rule is used to determine the

(1) Shape of molecule
(2) Number of bonds an atom forms

Reason

(A) The octet rule states that an atom forms covalent bonds through the sharing of electrons in order to have 8 electrons in the valence shell.

(B) The octet rule states that the number of bonds formed equals the number of electrons in the outer shell.

(C) The octet rule states that the shape of a molecule is dependent on the number of shared electron pairs.

(D) The octet rule states that the shape of a molecule is due to 4 electron pairs being located in tetrahedral positions.

8. If the compound OF_2 and CF_4 are compared, the strength of the intermolecular forces are

(1) Greater between OF_2 molecules
(2) Greater between CF_4 molecules
(3) The same for both types of molecules

Reason

(A) There are four polar bonds in CF_4 and only two in OF_2.

(B) The similar electronegativities of oxygen and fluorine result in OF_2 being non-polar.

(C) The large electronegativity difference between carbon and fluorine atoms results in CF_4 being polar.

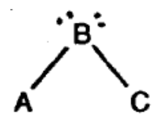
(D) CF_4 is symmetrical and non-polar, whereas OF_2 is non-symmetrical and polar.

9. The electron pair repulsion theory is used to determine the:

(1) Polarity of a molecule (2) Shape of a molecule

Reason

(A) Non-bonding electrons determine the polarity of a molecule. For example, non-bonding electrons on the atoms B in the molecule ABC cause B to become partially negative (δ^-).



(B) The theory states that the shape of a molecule is due to the arrangement of the bonding and non-bonding electron pairs around the central atom to minimize electron repulsion. .

(C) The theory states that the polarity of molecule id dependent on the number of polar bonds present

(D) The theory states that the shape of a molecule is due to repulsion between the atoms in the molecule.

10. The molecule SCl_2 has polar covalent bonds between the sulfur and chlorine atom. The atom assigned the partial positive charge (δ^+) in these bonds would be

(1) Sulfur (2) Chlorine

Reason

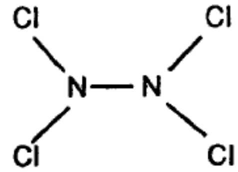
(A) The sulfur atom donates an electron to the chlorine atom resulting in the formation of S^+ and Cl^- Ions.

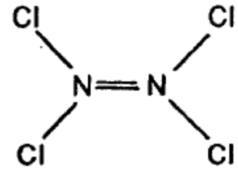
(B) The sulfur atom is partially negative (δ^-) as it can form as S^{2-} ion, whereas chlorine can only form a Cl^- ion.

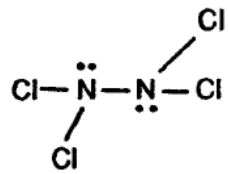
(C) The number of valence elections on the sulfur and chlorine atoms determine the polarity of the bonds

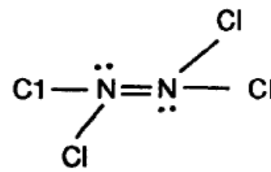
(D) Chlorine has the higher electronegativity and the shared electron pair tends to be located slightly closer to the chlorine atom than the sulfur atom.

11. Which of the following best represents the structure of the N_2Cl_4 molecule?

(1) 

(2) 

(3) 

(4) 

<u>Reason</u>

(A) The high electronegativity of nitrogen requires that a double or triple bond is always present.

(B) The structure is due to repulsion between the 5 electron pairs (including bonding and non-bonding pairs) of the nitrogen atom.

(C) The structure is due to repulsion between the 4 electron pairs (including bonding and non-bonding pairs) of the nitrogen atom.

12. Which of the following molecules is tetrahedral geometry?

(1) CF_4 (2) SCl_4 (3) $SeCl_4$

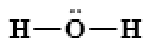
13. Which of the following molecules is linear geometry?

(1)  (2)  (3) 

14. Which of the following molecules are not polar?

(1) $BeCl_2$ (2) H_2S (3) CCl_2F_2

15. Given the Lewis structure of the following molecules, which of them is not polar?

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

APPENDIX E

THE INTERVIEW PROTOCOL

THE INTERVIEW PROTOCOL

Your participation is voluntary. What you will discuss in the interview won't affect your grade in any way. I am only interested in the process of your thinking, so do not worry about whether you get the questions right or wrong. If you are interested in finding out, we can discuss the textbook answers when the interview is done.

I want to understand what you are thinking when you solve these problems. For that reason, I would like you to talk your way through it. Please tell me whatever it is you are thinking, what image that you have in mind, and how you are working out each task.

Approximately 75 minutes; use to interviews high-scoring and low-scoring students

[Atomic model and valence electron]

Q1. The two diagrams below show things you might study in chemistry. Think about how the things shown in the diagrams are similar and how they are different (modified from Taber, 2002b):

F	Cl
Fluorine	Chlorine

In which ways are they alike?
In which ways are they different?

Please draw and describe to me how you think it would look like.
(If the participant mentions the number of overall electrons and valence electrons, probe for:
How are valence electrons different from the overall electrons?)

– probe for

- static mental image of atomic models
- number of overall electrons
- valence electrons
- electronegativity
- number of protons in the nucleus
- trends and groups in the Periodic table

[Bonding]

Q2. What does the term 'chemical bond' mean to you (adopted from Nicoll, 2001)?
Where (how) is the force exerted to keep the atoms together?
– probe for:

- word association
- intramolecular force

[Procedural knowledge and problem solving] (Think aloud)
Pretend that I am your classmate, and I know nothing about how to derive a Lewis structure and molecular structure from a chemical formula. So I need you to do your best to teach me and explain to me how you do that.

Q3. I have a molecule, H_2S, here. Please explain to me how you would derive its Lewis structure and molecular geometry.

For Lewis structure, probe for:

- use of the Periodic table
- number of valence electron
- octet rule
- bond type
- lone pair electrons

Explain to me why you drew it that way.
What does each part of the Lewis structure (octet rule, bonding, lone pair electrons) mean to you?

Based on the representation that students used to derive molecular geometry, probe for:

- octet rule
- bond type
- lone pair electrons
- VSEPR theory or hybridization
- repulsion
- explanation about its molecular geometry (3D spatial arrangement)
- description about its repulsion between S-H bonds

What image in your mind helps you to determine its structure?
Please build the molecular model of H_2S using the Play-dough and straws in front of you (adopted from Nicoll, 2001)
Please explain to me why you built the molecule the way you did – molecular shape

[Microscopic representations] (modified from Nicoll, 2001)
Q4. If you could zoom in to on the sample until you can only see a single molecule of H_2S, what would you see?
Please explain to me why you would see that.

– probe for:

- bonding/bond type
- region of electron density
- motion of electrons
- motion of molecules

Does that look the same as the model you built? If not, how is that different?
Is it a static image or is it in a constant motion? Please describe.
What properties about the molecule make it behave that way?

Q5. Now we're going to zoom in on that molecule of H_2S until you can see what's going on inside the molecule. Describe what you would see?
Where are the electrons in the molecule?
How are the electrons distributed around the molecule?
Explain how and why the electrons are shared.
How are the lone pairs of electrons different from the shared pair of electrons?
Do you think that this is a complete representation of your understanding of these concepts? Why?

[Molecular polarity]
Q6. Is H_2S a polar or non-polar molecule? Please explain.

– probe for:
- geometry (e.g., symmetric structure, 3D spatial arrangement)
- polar/non-polar bond
- electronegativity
- bond moment/direction of bond moment(s)
- Dipole moment (vector quantity)

Please explain which part in the diagram you draw (or the model you built) makes the molecule polar?
What would be the bond angle between S–H bonds? Please explain.
Do you use the image in your mind to help determine if it is polar or non-polar? How?
Is your drawing the same as the image that you have in your mind? How is that the same (or different)?

Q7. Is BF_3 a polar or non-polar molecular? Please explain.

– probe for:
- geometry (e.g., symmetric structure, 3D spatial arrangement)
- polar/non-polar bond
- electronegativity
- bond moment/direction of bond moment(s)
- dipole moment (vector quantity)

What image helps you to determine its structure?
Please explain which part in the diagram you draw (or the model you built) makes the molecule polar?
What would be the bond angle between B–F bonds? Please explain.
Do you use the image in your mind to help determine if it is polar or non-polar? How?

Q8. What does the term “polar molecule” mean to you?
If you have a bunch of polar molecules, how do these polar molecules behave?
How do a bunch of non-polar molecules behave?
Please give me another example of non-polar molecule.

[Electronegativity]

Q9. How would the bond angle change if the two H are replaced with two Cl? Explain why.

H_2S SCl_2

– probe for:

- geometry (e.g., symmetric structure, 3D spatial arrangement)
- electronegativity
- bond moment/direction of bond moment
- repulsion
- the change of region of electron density
- polar/non-polar bond
- dipole moment (SCl_2 is more polar or less polar?)

What image helps you to answer this question?
What does the image look like? Please draw or build a model to explain.
Please explain to me how you use the image in your mind to think about this question.
If you were to build a model for SCl_2, how would the model differ from the model of H_2S that you have built earlier?

APPENDIX F

DATA COLLECTION MATRIX

DATA COLLECTION MATRIX

Overarching Research Question: What are the influences on students' problem-solving about molecular polarity?

Research questions \ Data sources	Responses of instrument EN, CB, and GP	Interview and video-taping	Artifacts
What mental-modeling ability do high-scoring, moderate-scoring, and low-scoring students possess regarding molecular polarity?	S	P	P
What conceptual framework do high-scoring, moderate-scoring, and low-scoring students possess regarding molecular polarity?	S	P	P
What mental models do high-scoring, moderate-scoring, and low-scoring students construct regarding molecular polarity?	S	P	P
What contributes to the differences between high-scoring, moderate-scoring, and low-scoring students on their understanding of molecular polarity?	S	P	P

P=Primary data source used to answer the research questions; S=Secondary or supporting data source used to answer the research questions

VITA

Chia-Yu Wang grew up in Taipei, Taiwan, where she completed her elementary and secondary education. She received a Bachelors of Science in Applied Chemistry from National Chiao Tung University in Hsinchu, Taiwan. While Chia-Yu received a Masters of Science in Materials Science and Engineering, she completed educational courses for secondary certification from National Chiao Tung University. She worked as an engineer in industry before she decided to pursue her doctoral degree in science education.

After spending her first year of the doctoral program in science education at Texas A&M University, Chia-Yu transferred to the University of Missouri-Columbia (MU) to continue her degree in science education program. Dr. Lloyd H. Barrow is her program advisor and dissertation chair. She is currently working as a graduate research assistant for a state-funded professional development evaluation grant. During her four years at MU she worked with her advisor, Dr. Barrow, and committee members, Drs. Abell, Volkmann, Ehlert, and Robertson on various research projects in science education. Chia-Yu developed a strong collegial relationship with her advisor and committee members over the years through various research experiences.

In August of 2007, Chia-Yu will go back to Taiwan and hope to receive an offer of an assistant professor position in science education at National Chiao Tung University. Her future teaching and research foci will remain on improving teaching and learning chemistry at secondary and undergraduate levels.