STUDENTS' UNDERSTANDING OF STRUCTURE-PROPERTY RELATIONSHIPS AND THE ROLE OF INTERMOLECULAR FORCES

By

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ABSTRACT

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The connection between the molecular-level structure of a substance and its physical and chemical properties (such as boiling point or relative acidity) is an integral chemistry concept and a thorough understanding of this relationship is key to understanding larger and more complex chemistry ideas. Previous research has shown that students possess a wide range of non-normative ideas about chemical and physical properties. Student difficulties with the connection between a chemical structure and the properties of the compound, however, are far more complex than a series of misconceptions. Using a qualitative approach, we interviewed seventeen students enrolled in either general or organic chemistry courses. We found that, while many students could correctly predict and rank melting and boiling points of various compounds, few successfully used the molecular level structure of each compound to predict and explain its properties. Instead, we identified several emergent themes that categorize the ways in which students tried to explain these trends. While some students discussed similar individual ideas, no two students connected these ideas in the same manner, resulting in a wide range of interconnected, albeit fragmented, ideas.

Intermolecular forces (IMFs), the forces that govern interactions between molecules based on differences in polarity and electronegativity, play an important role in this connection between structure and properties. Because few students discussed IMFs when describing the connection between structure and properties in our interviews, we designed the Intermolecular Forces Assessment (IMFA) to specifically explore students' understanding of IMFs using questions requiring both written responses and drawn representations. This assessment was given to several groups of students at various time points at two different universities. We found that the modality of a student's response (e.g. drawing or writing) provided different insight into student understanding. Surprisingly, students' written descriptions of IMFs did not always align with their provided representations and analyzing the writing alone would have given a false impression of their understanding. Constructed representations, however, often provided crucial spatial information needed to determine if the students understood IMFs as occurring between molecules rather than within molecules.

Using the IMFA, we also studied the effect of an alternative general chemistry curriculum, Chemistry, Life, the Universe, and Everything (CLUE), on students' understanding of IMFs. Using two matched groups of students, those enrolled in the CLUE course and those enrolled in a traditional general chemistry course, we found that CLUE students most often correctly represented IMFs as occurring *between molecules* unlike the majority of students enrolled in traditional general chemistry courses who incorrectly represented IMFs as forces *within a single molecule*. We replicated these findings with an additional cohort of students the following year and have preliminary data that suggest these results extend to an additional university and are more generalizable.

While students' drawing can certainly be illuminating when exploring their understanding, analysis of student drawings is not always practical in terms of assessment. We investigated the use of automated text analysis of students' IMFA responses to explore its effectiveness in determining students' ideas about IMFs. We include preliminary findings using automated analysis of students' written responses to attempt to predict the drawing code a student would receive for their corresponding constructed representation of a specific IMF. This dissertation is dedicated to my loving husband Benjamin Williams. He was there to see me off as I started my graduate school journey in South Carolina, he supported me from afar when my educational pursuits sent me to Michigan, and he has patiently listened to me bemoan writing this dissertation (even though I am certain that my whining was extremely annoying). He has provided unwavering love, support, and understanding throughout this entire process and I am forever grateful. I would also like to dedicate this dissertation to my wonderful family. I certainly would not be the person I am today if not for them. They have always supported my pursuits, academic or otherwise, and have provided love and guidance in the best and worst of times. This one's for y'all.

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CHAPTER I: INTRODUCTION

Isolated material particles are abstraction, their properties being definable and observable only through their interaction with other systems. - Niels Bohr¹

Understanding the relationship between a structure and its resulting function is a key concept for various STEM (science, technology, engineering, and mathematics) disciplines. The National Research Council has repeatedly highlighted the importance of emphasizing this relationship in their previous science education standards² as well as listing it as one of seven crosscutting concepts in their recently released Framework for K-12 science education.³ This understanding of structure-property relationships plays a particularly important role in the study of chemistry. Much of what we expect students to learn in their introductory chemistry courses relates to and builds off of this understanding. Specifically, the knowledge that the molecular structure can influence the properties we experience at the macroscopic level, such as boiling and melting point or reactivity, serves as a solid foundation that students can use as they expand their knowledge of chemical phenomena.

Unfortunately, we know from previous research that students struggle to make this connection between the molecular structure of a substance and its resulting properties.^{4–6} Understanding this relationship requires thorough knowledge of a variety of interconnected topics and rules that build off of each other, as shown in Figure 1.1.⁶ The complexity of this connection can make it difficult for students to see the molecular structure as a tool to predict and explain properties. Instead, they often resort to memorized rules and heuristics to determine the properties of a substance without considering the key underlying chemical concepts.^{4,7,8}



Figure 1.1: The sequence of topics required to connect a given molecular formula of a compound to its resulting physical and chemical properties. Reproduced with permission of The Royal Society of Chemistry.⁶

Intermolecular forces (IMFs) play an important role in bridging the connection between molecular structure and the properties of a substance. Resulting properties, such as relative boiling or melting points, often depend on the type and strength of IMFs exhibited by a particular compound. These IMFs are influenced by the arrangement and electronegativity of elements within a given structure. Previous research has shown that students possess a range of alterative ideas and conceptions about IMFs, where they are located, and how they affect a compound's properties.^{9–11} It should come as no surprise then that students who struggle to understand IMFs also experience difficulties in explaining and predicting chemical and physical properties.⁴

Main Goals and Research Questions

The research presented here is a continuation of a series of projects centered on students' understanding of the connection between structure and properties.^{5,6,12,13} Our previous work has shown that students struggle to construct Lewis structures¹² and often do not understand their

purpose as tools to predict the properties of a given substance.^{5,6} Continuing in this vein of research, our first main goal, explored in Study 1, was to determine if and how students connect the molecular-level structure of a substance to its properties. Specifically, our research questions were:

Study 1

RQ1. In what ways do students use molecular-level structures to make predictions about the macroscopic properties of a substance?

RQ2. How do students enrolled in general and organic chemistry use representations of chemical structures to make predictions about macroscopic properties of substances?

Based on the broad nature of our research questions and the need for more detailed student responses, our data derives from a series of seventeen semi-structured interviews conducted with students enrolled in either general chemistry or organic chemistry. We collected both audio recordings of the interviews as well as any student drawings or written work for analysis. These interviews allowed us to approach the topic from a variety of angles and ask follow-up questions to students' responses for further clarity. Through open coding of our interview data and the refinement of our codes, we were able to identify several main themes (including representational difficulties and use of heuristics in student reasoning) that governed the ways in which students thought about and discussed the relationship between structure and properties.⁴

When analyzing these interviews, we noticed glimpses of students' understanding of IMFs, however the majority of students did not use these IMFs to help explain relevant physical and chemical properties. Instead they often relied on heuristics and memorized trends. The students who did discuss IMFs often did not elaborate on their understanding or provided superficial descriptions. Therefore, we wanted to collect responses from a larger group of students to further explore this topic as well as improve the generalizability of our findings. The main goals of this research were to develop an understanding of how students discuss and represent IMFs (Study 2) as well as to study the effects of an alternative general chemistry curriculum, *Chemistry, Life, the Universe, and Everything* (CLUE)^{14,15}, on students' ideas of IMFs (Study 3). Our specific research questions were:

Study 2

RQ1. How do students represent IMFs in free-form drawings? *RQ2*. How do students discuss and describe IMFs in open-ended written responses?

RQ3. How do students' written explanations compare to their drawn representations?

Study 3

RQ1. How do CLUE students' representations of IMFs compare to students enrolled in a traditional general chemistry course?

RQ2. How do students at different institutions compare in their representations of IMFs?

RQ3. How do CLUE and traditional students' representations of IMFs change over the course of the subsequent organic chemistry course?

The data for Study 2 and Study 3 come from the Intermolecular Forces Assessment (IMFA), a nine question assessment requiring students to both answer open-ended questions about their understanding of IMFs as well as construct representations of specific IMFs. We developed this assessment, as outlined in Chapter 5, based on our previous findings from Study 1 and our desire to incorporate both drawing and writing into a single assessment to explore students' understanding of IMFs. We collected responses from three different cohorts of students across two universities for comparison. We also followed a small group of students longitudinally though two years of introductory chemistry courses, from general chemistry to organic chemistry, to study the change, or lack thereof, in their understanding of IMFs over time. From the coding of both students' drawing and writing, we were able to compare their responses in both modalities to assess the effectiveness of each in determining their understanding of molecular interactions.⁹

While analyzing students' constructed representations of IMFs from the IMFA provided a wealth of information about their understanding, the process of coding hundreds of student drawn responses by hand is not entirely practical. Often instructors do not have the time or resources to dedicate to the analysis of open-ended written or drawn responses, thus the appeal of multiple-choice assessment items. Our third main goal for this research, explored in Study 4, was to investigate ways of expediting the analysis of IMFA written responses to glean as much information as possible without tedious and time-consuming hand coding. Specifically, our research questions were:

Study 4

RQ1. How well does lexical analysis of students' written descriptions of hydrogen bonding predict the location of hydrogen bonding in their constructed representation?

RQ2. What impact does an alternative general chemistry curriculum have on students' written IMFA responses? That is, can lexical analysis of written responses differentiate between students enrolled in different curricula?

The data for Study 4 come from students' responses to the IMFA collected at two different universities for three different cohorts of students. Key terms used in students' written responses were identified using lexical analysis and then used in a text analysis software system to build a model via discriminant analysis to predict the drawing code applied to a student's constructed representation in the IMFA. We also attempted to predict students' enrollment in either the CLUE general chemistry curriculum or the traditional general chemistry curriculum by using discriminant analysis of their written responses. REFERENCES

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CHAPTER II: THEORETICAL FRAMEWORKS

Nobody thinks clearly, no matter what they pretend. Thinking's a dizzy business, a matter of catching as many of those foggy glimpses as you can and fitting them together the best you can. - Dashiell Hammett, *The Dain Curse*¹

The history of educational research reaches back to the nineteenth century when researchers began to use scientific methods to systematically explore how people learn.² These early studies have their roots in behaviorism, spearheaded by the works of Edward Thorndike. Learning was viewed as behavioral in that it could be manipulated and controlled based on applied influences, what Thorndike called the Law of Effect.³ While behaviorism in the early twentieth century studied learning through the creation and alteration of engrained behaviors, researchers at the time had difficulty expanding these studies to explore thought and reasoning processes. The 1950's saw the rise of the multidisciplinary field of cognitive science where emphasis was placed on understanding human thought processes through new rigorous methodologies. Using these new methodologies, researchers were able to formulate and test theories of learning.²

Constructivism and meaningful learning

With the rise of studies on learning and human understanding came an additional emphasis on the process of *knowing*, that is, what factors influence the gaining of new knowledge and how its subsequently applied to novel situations. To better understand this focus on the process of knowing, we have to consult the work of researchers such as Piaget and Vygotsky. Piaget provided the foundation on which much of constructivism, as we know it

today, was built (although he was not the first to suggest the idea⁴). He reasoned that intelligence in children develops ontologically, and he should therefore be able to observe and research its development.⁵ Piaget's work, in fact, was framed in contrast to the idea of behaviorism and stimulus-response theory. He studied children over several years and concluded that children were actively involved and responsible for their own mental development as they tried to make sense of the world around them.⁶ Piaget emphasized the importance of a child's actions and their individual interpretations of those actions:

Learning is possible only when there is active assimilation. It is this activity on the part of the subject which seems to me to be underplayed in the stimulusresponse schema...All the emphasis is placed on the activity of the subject himself, and I think that without this activity there is no possible didactic or pedagogy which significantly transforms the subject.⁵

Vygotsky held similar views but also emphasized his idea of the zone of proximal development, which represented the distance between the learner's current level of knowledge and the level they could achieve through instructor guidance.⁷ He argued that learners could only truly understand material appropriate for their developmental level. For example, it may be appropriate for high school students with a general science background to take an introductory chemistry course, but place them in a graduate-level physical chemistry course and they most likely would understand little to none of the material. The most effective learning would then take place in the learner's zone of proximal development, which is entirely dependent on their current knowledge level.

Constructivism has since expanded into a variety of theories of knowledge⁸ such as social constructivism⁹ and radical constructivism.¹⁰ In its most basic form, however, it can best be described by the idea that "knowledge is constructed in the mind of the learner."⁶ One major critique, however, is that constructivism is a theory of learning rather than a theory of instruction.² That is, pure constructivism discounts the role of instructors and their influence when it comes to the development of new knowledge.⁸ With this in mind, it is useful to consider the theory of meaningful learning.

Meaningful learning finds its origins in the works of David Ausubel and his assimilation theory.¹¹ He first described meaningful learning as occurring when the learner chooses to incorporate new knowledge purposefully into their already existing framework of knowledge through "non-arbitrary relationships" in contrast to rote learning, which he described as approaching knowledge as small, isolated units of information that have no explicit anchoring to prior knowledge.^{12,13} Because individuals differ greatly in their knowledge structures and efforts to integrate new knowledge, however, meaningful learning and rote learning should be considered as a continuum rather than dichotomous.^{14,15} Unfortunately, much of traditional school learning occurs at the rote-learning end of the continuum. While rote learning can be preferable in certain circumstances, such as learning a new language or memorizing multiplication tables, there is often not enough emphasis placed on meaningful learning. A beneficial example of meaningful learning in the classroom would be an emphasis on the relationship between two concepts.¹⁶

In order for meaningful learning to occur, three basic tenets must be met: the learner must possess some relevant knowledge to which they can connect the new knowledge to, the new knowledge must be meaningful to the learner and presented in a meaningful way by the

instructor, and the learner must then choose to learning meaningfully as opposed to undergoing rote learning.¹⁷ These requirements for meaningful learning are outlined below in Figure 2.1. Students who undergo meaningful learning often remember information longer due to the increase in neural connections. Studies have shown that information learned via rote learning is typically forgotten within six to eight weeks.¹⁶



*Figure 2.1: Concept map of the requirements for meaning learning*¹⁷

Identifying prior knowledge: Moving beyond misconceptions to p-prims

We certainly understand that students enter the classroom, be it science or otherwise, with a set of ideas and preconceived notions that are often at odds with what we understand to be true.¹⁸ One prevalent theory in education research is the idea that all students possess misconceptions, or deeply entrenched and stable false ideas and beliefs.^{19,20} To overcome misconceptions, instructors should help students confront their misconceptions with contradictory knowledge and facts in order to produce conceptual change, that is, the reorganization or replacement of central concepts.²¹ In order for conceptual change to be effective, however, diSessa argued that the misconceptions students' posses would have to be few and "amenable to attack with data and argument", otherwise it is doubtful that confronting these ideas would produce the desired result.²² Additionally, diSessa points out, "there are, in fact, no widely accepted, well-articulated, and tested theories of conceptual change."²³

While most misconceptions literature typically focuses on the coherency of student understanding, researchers like diSessa argue that learners possess fragmented pieces of knowledge, called phenomenological primitives (p-prims) or facets. These facets of knowledge are phenomenological in nature, meaning they arise from an effort to make sense of natural events; they are primitive in that they are often offered up as self-explanatory and require no justification.²² Unlike the coherency stressed in theories of conceptual change, p-prims are loosely woven and highly fragmented.²⁴

diSessa describes a variety of p-prims, most based in physics, in his work. For example, he discusses the musical bells used as Montessori educational tools to highlight the "more x begets more y" p-prim.²² While the bells vary in pitch, they all appear to be the same size and made of the same material. So how do the bells produce different pitches? Most people will say

that the bells must vary in thickness. While this is true, the question then becomes which results in a higher pitch, the thicker or the thinner bells? Here is where p-prims tend to come into play as intuitive reasoning. The most common answer is that thicker bells produce lower pitches (which is the opposite of what actually occurs), however few can explain *why* they believe this to be true. Intuitively, it feels like the right answer; thicker/bigger/heavier things produce lower pitches. diSessa lists this idea under the larger p-prim "more *x* begets more *y*".²² In this sense, the p-prim becomes more generalizable to other areas of study.

For an expert, diSessa states that a discussion of pitch would trigger the concept of vibration, which would trigger the knowledge of a simple harmonic oscillator. As a result, the expert may conclude that, while a thicker bell would be heavier, it would also be stiffer. diSessa argues that experts also use intuitive p-prims when initially approaching problems, like "stiffer implies faster". The main difference, however, is that experts know when to appropriately use these ideas as guides, and they can justify them if need be with additional content knowledge.²² Novices, however, have more difficulty integrating new knowledge and, therefore, it is with an understanding of these processes that we can continue to inform and influence theories of learning.

How we learn: Working memory and information processing

Alan Baddeley was one of the first to suggest the theory of working memory during the late 1960's. Working memory, while often inappropriately considered synonymous with short-term memory, refers to a system of the brain used for temporary information storage *and manipulation*.²⁵ This system is vital for cognitive processes such as learning and comprehension. Unfortunately, this space is rather limited and can easily be overwhelmed.²⁶ For instance,

extreme performance pressure, such as completing mathematics problems on an exam, can consume working memory space and make it more difficult to perform well.²⁷ Johnstone provides a succinct model of working memory as part of the information processing model, shown in Figure 2.2, that allows us to analyze the factors that affect working memory and how it relates to long-term memory (LTM).^{28,29}



Figure 2.2: Johnstone's information processing model and working memory^{28,29}

Learners are constantly experiencing external information and events, which can certainly be overwhelming. This is best explained in terms of multimedia learning theory, which describes the human information processing system as having dual channels for sensory input: verbal and pictorial.³⁰ These two inputs are processed in the working memory space, resulting in limited capacity and the learner can switch a representation from one format to another for processing.³¹ For instance, when sitting in a chemistry lecture course students are often exposed to a verbal lecture from the professor, a visual display of information (typically through Powerpoint slides), and even their own written notes or textbooks for additional information. A student may listen to the lecturer describe the interactions of molecules and mentally convert the words to a picture, changing the processing type from verbal to pictorial. Multimedia learning stresses the idea that "in the process of trying to build connections between words and pictures, learners are able to create a deeper understanding than from words or pictures alone."³¹

When presented with a variety of information and sensory inputs, learners must filter out extraneous information in order to take in relevant information. Often what they decide to keep or filter out is influenced by knowledge already stored in their LTM. Obviously, this arrangement benefits experts and those with a more robust and knowledgeable LTM who are better able to recognize and filter out extra, unnecessary information. Once new information enters the working memory space, it can interact with information stored in the LTM to facilitate learning and successful incorporation into the LTM. As mentioned previously, this space is limited, easily overwhelmed, and, as a result, can make learning difficult.²⁶

Cognitive load theory (CLT) combines the discussion of LTM and working memory with the idea of automatic processing. The theory describes how schema developed in LTM can be used in working memory to allow for more efficient processing of data.^{32,33} For example, continued practice solving sets of algebraic problems (like (a+b)/c=d, solve for a) can lead to the development of schema that make addressing these problems easier and faster over time. The learner will become more familiar with these types of algebraic problems and will be better able to recognize and solve increasingly more complex versions of these problems.³⁴

How we reason and make decisions: Heuristics and dual-process theory

There has been considerable evidence over the years that people employ heuristics to make quick, efficient decisions and avoid overwhelming working memory space. The idea of heuristics can be traced back to Simon's work in bounded rationality.³⁵ He proposed that individuals work within the confines of a given task as well as their own cognitive constraints.

Heuristics, therefore, are used to reduce the amount of cognitive effort expended and to simplify the decision-making process.³⁶ Unfortunately, while heuristics are certainly useful, they do not always lead to the correct answer. Shah and Oppenheimer have hypothesized that all heuristics, regardless of domain, most likely fall under a handful of larger heuristic types.³⁶ That is, even though some heuristics are task-specific, they are rarely domain-specific. The reasoning behind heuristic use becomes apparent when considering dual-process theory.

Dual-process theory was first suggested not long after Baddeley's studies with working memory.³⁷ The theory describes two systems of mind, System 1 and System 2, that explain how we reason.³⁸ System 1 processes are largely characterized by their autonomy, often resulting in these processes being described as reflexive and intuitive. System 2 requires deeper thought processes and can be associated with reasoning. It also typically invokes the working memory and is involved in hypothetical thinking. Cognitive decoupling, or the ability to separate real world representations from imaginary ones, is strongly linked to System 2 reasoning.³⁹ System 2 is correlated with higher performance on intelligence measures, unlike System 1, which appears to be independent of such measures. Stanovich⁴⁰ succinctly described System 1's function in problem solving:

...type 1 processing is 'quick and dirty'. This so-called heuristic processing is designed to get you into the right ballpark when solving a problem or making a decision, but it is not designed for the type of fine-grained analysis called for in situations of unusual importance...

Wason and Evans³⁷ first introduced the term dual-process theory in an attempt to explain why their research subjects seemed to be making specific choices based on a matching bias. They provided participants with four cards, like those shown below in Figure 2.3. Participants were asked which card or cards they would flip over to determine if the following statement was true or false: "if there is an A on one side of the card, then there is a 3 on the other side of the card."³⁹ Only 10% of their participants answered correctly (flipping card A and card 7). Instead, most participants elected to flip cards A and 3, essentially *matching* the terms discussed in the prompt rather than considering which cards could potentially negate the original statement. This experiment has been repeated by other researchers with the same results.⁴¹

AL	3	7
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Figure 2.3: Card experiment used by Wason and Evans to explore dual processes theory³⁹

Additional studies have shown, however, that when the context of the question changes and becomes more realistic, like comparing ages on one side of the card with alcoholic or nonalcoholic beverage choices on the other side, the answer becomes significantly more obvious to participants.⁴² In terms of dual-process theory, it is hypothesized that abstract versions of the question, like Wason's original problem, require logical reasoning to solve (System 2) and thus many individuals do not perform well. Revised versions of the question set in a familiar context, however, appear to lead participants to the correct conclusion automatically without much reasoning (evoking System 1).⁴³ Often, the way a question or problem is worded can prompt an automated, System 1 response over the use of System 2. For example, take the following problem from the Cognitive Reflection Test⁴⁴ (Version 1) and a rewritten version⁴⁵ (Version 2):

Version 1 – If it takes 5 machines 5 minutes to make 5 widgets, how long would it take 100 machines to make 100 widgets?

Version 2 – If it takes 5 machines 2 minutes to make 10 widgets, how long would it take 100 machines to make 100 widgets?

Each version of the question, in theory, is the same, but the variation in wording alters the approach that readers often take in solving the problem. In Version 1, a common answer is 100 minutes.⁴⁴ This response is considered a heuristic, System 1 response arising from an innate "feeling of rightness".⁴⁵ If the feeling of rightness is particularly strong, a System 2 override is deemed unnecessary, resulting in the instinctual answer prevailing. Even when participants are given extra time to solve a problem, shown using the Wason card experiment, participants spend more time trying to justify their initial choice (in this case the cards they were going to select) than they did considering the reasons for rejecting the remaining choices.⁴⁶

There has been some debate as to the terms System 1 and System 2 as they imply two individual, distinct systems. Rather, System 1 should ideally be plural as it encompasses several systems working in tandem, sometimes referred to as the autonomous set of systems (TASS).³⁹ In fact, many theories and terms for System 1 and System 2 have been subsumed under dual-process theory over the years as the theory has gained prominence. Evans lists several labels used instead of System 1 and System 2 in the literature that range from experiential, heuristic, and impulsive to systematic, analytic, and higher order.⁴⁷

Difficulties in the chemistry classroom: Representational competency

Up until now, the frameworks presented in this chapter have been broadly applicable to a range of fields of study. The majority of chemistry lies in the abstract, atomic realm where we cannot physically see the interactions and reactions taking place, only the resulting macroscopic physical and chemical changes. Johnstone describes this perfectly when he states "The common type of concepts with which children and adults are familiar are made up of tangible instances...But how about the concept of 'element' or 'compound'? There is no immediate sensory way to get at these ideas."²⁸ Because of its abstract nature, chemistry can be described using three levels of thought: macroscopic, microscopic, and symbolic (shown below in Figure 2.4).



Figure 2.4: Johnstone's Triangle of the three levels of thought. Reproduced with permission of John Wiley & Sons, Inc.²⁸

The macroscopic level encompasses that which we can see and feel, like changes in physical state. For chemistry, Johnstone described sub-microscopic as including molecular and atomic levels as well as forces and interactions.⁴⁸ Symbolic includes formulas and equations along with chemical structures and graphs. While understanding each level alone can be complicated, most often chemistry concepts reference all three levels simultaneously with
different degrees of emphasis. For example, hydrogen bonding is often introduced by discussing the macroscopic concept of boiling water and explaining that the temperature at which water boils is directly related to the strength of the attractive forces between water molecules (submicroscopic), which can be determined based on the molecular structure (symbolic) and geometry. While experts may be able to fluidly transition between these levels, for students this can be a particularly difficult challenge.

Some believe that chemistry places too much emphasis on the interplay of the symbolic and submicroscopic levels, with less reference to the macroscopic level.⁴⁹ Because of the abstract nature of chemistry, there is a heavy reliance on the use of representations to convey ideas that cannot be experienced first-hand. Kozma and Russell⁵⁰ define representational competence as "a set of skills and practices that allow a person to reflectively use a variety of representations or visualizations...to think about, communicate, and act on chemical phenomena in terms of underlying, aperceptual physical entities and processes."

Concluding remarks

Chemistry is notoriously considered by students to be one of the most difficult subjects of study. Its reputation is not necessarily unfounded. Many students struggle to grasp the complex and abstract nature of chemistry and often, introductory chemistry courses sacrifice depth of material for breadth. The ways in which chemistry has been taught over the years has not aligned well with what we know about learning and integration of new knowledge. Take the complex relationship between structure and properties. In order to understand this connection, students must be fluent in Johnstone's three levels of thought; they should understand that representations could be used to show molecules and interactions as well as the macroscopic changes that result.

Meaningful learning tells us that instructors and the curriculum they use should be making these connections explicit for students, relating each step in the process back to the previous steps as well as highlighting the usefulness of each step in the overall process to determine macroscopic properties.

Instructors should also consider the prior knowledge that students bring with them to the classroom. Thinking is messy and as students attempt to sort through the plethora of new knowledge that they are exposed to, these ideas can become fragmented and loosely woven together in an attempt to build reasonable explanations. While these ideas at times can be persistent and difficult to change, providing a strong base of essential chemical concepts, perhaps through learning progressions^{51,52}, can result in a solid foundation from which students can build and integrate new knowledge. Assessment plays an essential role in determining what students' have learned. By understanding heuristic use and dual-process theory, instructors should be mindful to create questions that force students to override their impulsive, System 1 processes and use System 2 to develop rational and analytical responses. Assessment items that can be answered through the use of heuristics and other short cuts fail to engage System 2 processes involved in deeper, rational thought. By identifying students' prior knowledge, explicitly connecting new concepts to foundational knowledge, and designing effective assessments, instructors can have a positive impact on students' understanding of chemistry concepts.

Several of these frameworks have guided the research presented in this dissertation. Because of the complexity of students' understanding of the relationship between structure and properties, we chose to analyze and dissect our structure-property interviews through the lens of dual process theory and p-prims. Our work with students' representations, both in our interviews and with the Intermolecular Forces Assessment (IMFA) was influenced by studies on

representational competence in chemistry and the interplay of words and pictures outlined by multimedia learning theory. Finally, our exploration of the effects of a reformed curriculum on student understanding highlight the need to thoughtfully design curricula to reflect the tenets of meaningful learning.

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CHAPTER III: A REVIEW OF THE LITERATURE ON STRUCTURE-PROPERTY RELATIONSHIPS AND INTERMOLECULAR FORCES

All things are made of atoms — little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied. - Richard Feynman, 1977¹

The relationship between structure and property

The idea that the structure directly influences function is an integral scientific concept. I say scientific rather than chemical because that single statement applies to a wide range of scientific fields. In biochemistry, the shape of a protein determines its function, and in biology the structure and composition of leaves allow them to collect sunlight for photosynthesis; in physics (and even engineering) the structure and design of wings allow for flight. While this concept can be succinctly described in a few sentences, it encompasses a vast array of information.

In terms of chemistry, the relationship between structure and function is best highlighted by the idea that the physical and chemical properties of a substance can be traced back to the molecular level structure of the molecules that make up that substance and their interactions. We know that students struggle with this relationship and understandably so.^{2–5} In order to make this connection, students have to complete a long chain of inferences. They must be able to construct a representation of the molecule (typically a Lewis structure), identify its geometry and shape,

use their understanding of electronegativity and bond polarity along with shape to determine molecular polarity, identify the type and strength of intermolecular forces that the molecule is capable of, and finally combine all of this information to predict the physical and chemical properties the substance might exhibit.²

Each of these steps alone can be daunting for students. We know, for instance, that students have trouble constructing Lewis structures and often are not aware that they can be used to predict chemical and physical properties.^{2,6,7} Shane and Bodner interviewed three students and described the inability of one student to view Lewis structures as symbolic rather than verbo-linguistic (a set of lines, letters, and dots with no symbolism).⁸ If students cannot construct the correct molecular structure, or do not know what Lewis structures are for, then we should not be surprised when they cannot use the structure to predict properties.

DeFever and colleagues have reported that students rarely discuss shape and geometry when determining the polarity and resulting solubility of different compounds.⁵ A study by Birk and Kurtz as well as one by Peterson and colleagues both identified similar student misconceptions related to polarity. They both found that students often ignored molecular shape and felt molecules could only be nonpolar if the atoms within the molecule had the same electronegativities.^{9,10} While identifying the elements present can help students determine the polarity of a molecule, the geometry and shape of the molecule play an important role. For instance, while carbon dioxide contains polar bonds, its linear shape allows for the resulting nonpolar molecule.

Students' understanding of physical and chemical properties

Several studies have explored students' ability to predict relative chemical or physical properties of various compounds. Talanquer and colleagues investigated how students predict reactivity and acidity for a group of compounds and found that they relied on heuristics and trends to inform their decisions.^{11,12} DeFever and colleagues described students' difficulty predicting the reactivities of compounds when the structures provided were less familiar to them. They reported that students often tackled these structures by comparing them to other structures they were familiar with, essentially scanning their "mental rolodexes" until they found a structure that they believed to be a suitable match.⁵

Students' understanding of various physical processes, like boiling and melting, is also well documented in the literature. For instance, we know that students have difficulties conceptualizing the idea of boiling or melting and often describe the process in terms of breaking covalent bonds within a molecule.^{4,10,13–15} Many studies have reported participants describing the composition of bubbles in boiling water as oxygen and hydrogen, indicating that students believe water molecules break up during the boiling process.^{16–19} Smith and Nakhleh explored students understanding of melting and dissolving processes for a variety of compounds (including salt, butter, and sugar) and found similar misconceptions of students breaking bonds or incorrect intermolecular forces during phase changes.¹³

Other studies have identified additional student ideas about phase and phase changes under the view of the particulate nature of matter, outlined by Nakhleh.²⁰ Griffiths and Preston interviewed grade 12 students and found several alternative ideas including the notion that water molecules change size depending on the phase of matter, that adding heat causes atoms to expand, and that water molecules in the solid phase are not bonded together in any specific

pattern.²¹ Othman and colleagues identified students who believed that the difference in a substance's phase could be related to the relative strength of the covalent bonds within the molecule.¹⁴ Other studies have explored how students explain physical processes such as boiling or melting in terms of IMFs, but before we discuss them, it would be beneficial to outline the concept of IMFs and the work that has been done on students' understanding of them.

Intermolecular Forces

Early chemical theory, suggested by Empedocles and refined by Aristotle, stated that there were "only two fundamental forces to account for all natural phenomena. One was Love, the other was Hate. The first brought things together while the second caused them to part."²² As romantic as this notion may be, we now understand there to be four fundamental forces: strong, weak, electromagnetic, and gravitational. The idea that there are attractive forces that exist between particles and govern macroscopic properties was not addressed quantitatively until in the mid-1700's and even then was often thought to be influenced by gravity.²³ There was little discussion as to what might be causing these hypothetical interactions.

The concept of intermolecular forces (IMFs) has expanded and morphed since then, but the original idea remains the same: there exist non-covalent interactions between molecules (and sometimes within very large molecules) that are governed by differences in charge. The most common intermolecular forces discussed in introductory chemistry courses are hydrogen bonding, dipole-dipole, ion-dipole, ion-induced dipole, dipole-induced dipole, and London dispersion forces (LDFs). The term van der Waals forces refers to a broader category of interactions, defined by the International Union of Pure and Applied Chemistry²⁴ as:

The attractive or repulsive forces between molecular entities (or between groups within the same molecular entity) other than those due to bond formation or to the electrostatic interaction of ions or of ionic groups with one another or with neutral molecules

For our purposes, we will focus mainly on hydrogen bonding, dipole-dipole, and LDFs. These three IMFs are predominantly emphasized in general chemistry curricula and are, therefore, of more interest to us. The key unifying idea behind these interactions, and the idea that we would hope most students would leave their introductory chemistry courses knowing, is that these interactions occur *between* small molecules and are responsible for a wide array of macroscopic physical and chemical properties.

Figure 3.1(a) - (c) shows common representations of the three main IMFs, hydrogen bonding, dipole-dipole, and LDFs, similar to those seen in *General Chemistry: Atoms First* by McMurry and Fay.²⁵ Hydrogen bonding is often represented as a dashed line between the lone pair of an extremely electronegative element and a hydrogen covalently bonded to another extremely electronegative element. Dipole-dipole interactions are sometimes also represented using a dashed line (as hydrogen bonding can be considered a stronger version of dipole-dipole) and often include partial positive and partial negative charges to indicate areas where these interactions occur. A variety of representations exist for LDFs, but most show either electrostatic potential maps or the distorted electron clouds of noble gas elements like helium or diatomic halogen molecules like iodine. These representations typically show one molecule with an instantaneous dipole that then induces a dipole on a neighboring molecule. Again representations

of LDFs often use the addition of partial positive and negative charges to show the dipoles responsible for the interaction.



Figure 3.1: Representations of (a) hydrogen bonding, (b) dipole-dipole, and (c) LDFs

Studies exploring students' understanding of IMFs

Many of the studies on students' understanding of intermolecular forces fall into one of two categories: studies about general IMFs^{10,26,27} or (more predominantly) studies about hydrogen bonding.^{28–33} For those studies that only generally explore IMFs, the main focus is often on the larger picture of chemical bonding rather than students' specific understanding of IMFs. Additionally, while many studies have reported misconceptions in students' understanding of hydrogen bonding, little work has been done to investigate how students' think about dipole-dipole interactions and LDFs.^{34,35} One possible reason for the focus on hydrogen bonding could be its unique role in biological systems or its association with the properties of water. The next sections will go into greater detail about these studies and their findings.

Intermolecular versus intramolecular forces: Students' understanding of bonding

Several researchers have explored students' understanding of IMFs in the context of bonding, as outlined by Özmen in his review of the chemical bonding literature.³⁶ Peterson and Treagust developed a two-tiered diagnostic instrument, which included two items about interand intramolecular forces. For these two items, 23% of students in grade 12 identified IMFs as forces within a molecule (rather than between molecules) and 33% of students cited IMFs as forces within a continuous covalent solid.¹⁰ Goh and colleagues administered the same diagnostic instrument to grade 12 students in Singapore and found similar results: 35% of students indicated that IMFs occurred within a molecule and 46% stated that they existed in a network covalent solid.²⁶

Coll and Taylor interviewed students at various levels (from high school to graduate school) and found additional alternative conceptions, such as the involvement of IMFs in ionic and metallic bonding as well as the notion that "intermolecular forces are influenced by gravity".²⁷ Griffiths and Preston also found students who hypothesized that water molecules may be held together by gravity or air pressure.²¹ Taber points out that when instructors discuss ionic and covalent bonding as two dichotomous ideas, there is little room for students to incorporate the concept of intermolecular forces. They are often either considered bonds or just a force.³⁷ While Taber and others argue for IMFs to be accepted as bonding, the difference between the two is still important to emphasize especially in terms of what happens on the molecular level during a phase change.^{37,38}

Student difficulties with hydrogen bonding

Other researchers have taken the exploration of students' understanding of the difference between intermolecular and intramolecular forces one step further and focused specifically on the conflation of hydrogen bonding with covalent bonding.^{28–30,32,33} Nicoll, in her interviews on Lewis structures and covalent bonding, found students who incorrectly identified covalent bonds within a formaldehyde molecule as hydrogen bonding.³⁹ Taber discussed this particular "alternative conception" in his book on chemical misconceptions. He argued that students are

first introduced to the idea of hydrogen bonding in biology, rather than in their chemistry course, and when instructors only mention the term without further discussion of its meaning, they can lead students astray.²⁸ While this may be true, it can also be argued that the term hydrogen bonding itself is misleading. Students' confusion with chemical terms like "atom" and "molecule"⁴⁰ or with words that possess everyday meanings like "pure"⁴¹ have been previously reported. It would certainly come as no surprise that intermolecular, intramolecular, and hydrogen bonding would lead to confusion as well.

Exploring students' understanding of hydrogen bonding through interviews and multiplechoice items

Most studies on IMFs, and hydrogen bonding specifically, rely on the use of either interviews or multiple-choice and written assessments to elicit student understanding. Schmidt and colleagues administered a multiple-choice assessment with follow-up short answer questions to over 3500 high school students. Their items related to IMFs required students to identify which compounds out of those provided (e.g. acetic acid, methyl fluoride, and dimethyl ether) would exhibit hydrogen bonding.²⁹ The assumption, however, is that students understand where hydrogen bonding occurs. Students are never asked to elaborate on the location of the IMF, but rather to identify compounds capable of hydrogen bonding. Henderleiter and colleagues made a similar assumption in their interviews of 22 organic chemistry students on hydrogen bonding, asking students to show were hydrogen bonds would form between given molecules. Again, there is an assumption that students understand IMFs as interactions *between* molecules.³⁰

Both studies explored the strategies and structural features used by students to determine hydrogen bonding. Schmidt and colleagues noted that some students determined if a compound

was capable of hydrogen bonding by simply identifying the presence of oxygen and hydrogen or by identifying the structural similarities to a known compound (like comparing dimethyl ether to water).²⁹ Henderleiter and colleagues found students who listed additional atoms as capable of hydrogen bonding (like carbon and sulfur) and students who confused intramolecular hydrogen bonding with a chemical reaction.³⁰

Similarly, Barker and Millar provided 250 students with Lewis structures of water interacting via dotted lines and asked them to explain both the dotted line between molecules and the solid line within a water molecule. At the end of their study, 24% of the population indicated that the dotted line was an attractive force (not a real bond). The researchers considered this statement inaccurate and coded it as evidence of partial misunderstanding, whereas referring to the dotted line as van der Waals or dipole-dipole bonds was considered evidence of partial understanding and identifying the interaction as hydrogen bonding with no explanation was considered evidence of understanding. While their coding scheme is somewhat unclear, they found that 68.4% of their population correctly identified the dotted line as hydrogen bonding by the end of the course.³¹

In a similar fashion, Villafañe and colleagues designed an instrument to uncover students' understanding of general biochemistry concepts. Three of the items on their assessment provided students with Lewis structures of carboxylic acids or amines with water and asked them to identify between which atoms hydrogen bonding would exist. Options included atoms within the same molecule (such as a covalent bond) and atoms between molecules (like oxygen on one molecule and hydrogen on another). Unlike other studies that explore this concept using multiple-choice exams, the authors did provided students the option to indicate hydrogen bonding as a bond within a molecule. Significantly, the questions relating to hydrogen bonding

resulted in the lowest Cronbach alpha value (0.306) out of all of their item sets indicating a weak correlation between students' responses to these items.³⁴

In a similar fashion, Nahum and colleagues asked students to indicate on a given diagram of several water molecules where hydrogen bonding would occur. Several students incorrectly identified where hydrogen bonding would occur, indicating interactions between incorrect atoms or covalent bonds within the molecule.³⁸ Assessment items, like the ones outlined here, most often require students to identify hydrogen bonding in a given representation or identify compounds capable of hydrogen bonding in the form of multiple-choice questions. They typically make several assumptions as to what a student does or does not know and are not necessarily accurate reflections of students' understanding of IMFs.

Drawing intermolecular forces

A small number of studies have required students to draw representations of hydrogen bonding to explore their understanding of this IMF. Pereira and Pestana were some of the first researchers to explore students' understanding of hydrogen bonding through drawings. The researchers asked Spanish high school students to construct representations of water as a solid, liquid, and gas. They found that most students failed to include a representation of hydrogen bonding in their drawings. For those students that did draw hydrogen bonding, some provided representations with bonds between hydrogen atoms on different molecules or even double bonds between molecules. Only eleven students out of the entire population (N=227) provided an "approximately correct" representation of "intermolecular bonds". It's important to note, however, that the authors placed a large emphasis on the portrayal of bond lengths and bond angles in students' drawings of water. If a student provided a representation of hydrogen bonding

between molecules but the length of the IMF was shorter than the bond length within the molecule, then the answer would be marked incorrect by the researchers.³²

Taagepera and colleagues asked general and organic chemistry students to draw representations of hydrogen bonding as part of a combination constructed-response and multiplechoice assessment. They found that the two most difficult items, averaging 36% and 40% correct responses, required students to draw IMFs; the first asked students to draw "the intermolecular interactions among these [methanol] molecules", the second to draw methanol molecules interacting with water molecules. Because the researchers were more interested in the connections students made between bonding concepts (like electronegativity and bond polarity), they spent less time characterizing students' representations of hydrogen bonding. They did note, however, that many students confused hydrogen bonding with a covalent bond and some inaccurately represented it as an interaction between hydrogens on different molecules.³³

Despite the work done with students' drawings in these two studies, little research has been done to explore students' understanding of IMFs through their constructed representations. Many studies make assumptions as to what students do and do not understand through the format and design of their assessment items and interview questions. With so few studies on dipoledipole and LDFs, additional research is still needed to explore these ideas in greater detail.

Intermolecular forces and their relationship to physical properties

In addition to exploring students' ideas and alternative conceptions about IMFs, several researchers have studied how students relate these IMFs to their understanding of physical properties, like boiling and melting points, and phases of matter. Ideally, students should be able to relate the type and strength of IMFs present to help them determine relative properties. For

example, stronger IMFs like hydrogen bonding require more energy to overcome resulting in higher melting and boiling points of a substance. Schmidt and colleagues asked high school students to predict which alkane, out of a series of increasingly branched alkanes, would have the lowest boiling point. Only 15% of the students who provided an explanation were able to connect surface area and van der Waals forces to the difference in relative boiling points. Other students explained the how the various structures effected the boiling point in terms of breaking covalent bonds, stability of the molecule, or the structure's ability to release H⁺ ions. The researchers acknowledge that, while they were able to identify alternative ideas about boiling, interviews with students would be necessary to further explore students' about on the process.²⁹

Henderleiter and colleagues explicitly asked students in their interviews to identify if the statement "the boiling point increases from methanol to ethanol to propanol is because of hydrogen bonding" was true or false and to explain why. They found that the majority of students interviewed correctly related the trend in increasing boiling points to the molar mass or chain length of the compounds. Other students only memorized the correct trend or explained it in terms of breaking covalent bonds or pKa. It's important to note, however, that the researchers never address if students effectively discussed that all three structures were capable of hydrogen bonding and that the increase in molar mass or chain length corresponds to more electrons, increased polarizability, and thus stronger LDFs which result in a higher boiling point. This connection is crucial and an indicator of coherent understanding, but it is unclear from the published study if students made this distinction.³⁰

Barker and Millar provided two substances to students, magnesium chloride and titanium (IV) chloride, and informed them that the first was ionic and the second was covalent. They then asked to students to explain why, upon heating a mixture of the two substances to 1000 °C, "the

resulting vapor consists only of titanium (IV) chloride". The intent was for students to explain that the IMFs between titanium (IV) chloride molecules are considerably weaker than the ionic bonds present in magnesium chloride and thus less energy would be needed to overcome them. The authors found that many students failed to discuss IMFs in their explanations of the boiling point of titanium (IV) chloride and instead readily attributed the lower boiling point to the presence of covalent bonds, sometimes indicating that the covalent bonds themselves would break. Barker and Millar also noted that the format of the question might have influenced students' responses. By explicitly stating that one substance was ionic and the other covalent, it may not have been apparent to students that a discussion of IMFs was necessary to successfully answer the question.³¹

Few studies have explicitly and intentionally explored students' understanding of the role of IMFs in determining various physical properties. For those that have, responses alluding to molar mass or chain length were accepted as evidence of students' understanding of the role of LDFs in determining boiling and melting points. There was little discussion of *how* chain length and boiling point are connected. Additionally, as we saw with Barker and Millar's study, question wording can affect the ways in which students respond in their explanations. More work is certainly needed to explore if students understand that IMFs, not chain length or covalent bonds, affect the relative boiling and melting points of compounds.

Attempts to improve students' understanding of IMFs

While it is necessary to identify students' difficulties with the relationship between structure and properties and the role of intermolecular forces, it is also important to discuss evidence-based solutions to address these problems. Proposed solutions reported in the literature range from small intervention activities and lab projects to full redesign of chemistry curricula. Many authors have suggested short examples to help students better understand IMFs, such as doing the "wave" to mimic LDFs⁴², using magnets to represent dipole-dipole interactions⁴³, or even using a structural database to model intermolecular interactions⁴⁴. Most of these examples, however, are intentionally designed as helpful suggestions with no evidence to support their effectiveness. Few studies cite improvement in students' understanding of IMFs, and many have issues with methodology or analysis.

Tarhan and colleagues studied the effects of active learning on students' understanding of hydrogen bonding, dipole-dipole and LDFs by incorporating problem-based learning (PBL) activities into the classroom. The researchers found statistically significant differences between their treatment and control groups on post-test questions related to IMFs and stated that "students in the PBL group had no alternate conceptions about intermolecular forces." Unfortunately, the post-test included items like "In which of the H₂O and CH₄ molecules does hydrogen bonding occur? Explain." and "Which of the N₂, HCl, and NH₃ molecule/molecules have dipole-dipole forces? Explain." As discussed previously, questions that require students to identify compounds capable of IMFs may not accurately reflect student understanding of IMFs. It was also unclear how researchers determined correct or partially correct responses.³⁵ Problem-based learning has been used in other areas to aid student understanding⁴⁵, and that may certainly be the case here, but additional evidence is needed to support the authors' claim.

Ealy attempted to use molecular modeling in the lab to improve students' understanding of IMFs. The author found statistically significant differences between treatment and control groups on post-test assessment items. Ealy chose to use multiple-choice assessment items to test students' understanding but, like Tarhan and colleagues, included questions that asked students

to identify the strongest IMF present for three different compounds. Ealy also conducted statistical analyses on rather small sets of treatment and control groups (Group 1: N=23 and N=23; Group 2: N=33 and N=33) and failed to include effect sizes, which would be a better indicator of the magnitude of the effect.⁴⁶ Again, the assessment items included here may not be successful at uncovering actual student understanding of IMFs, and thus it is difficult to determine the effectiveness of these molecular modeling activities.

Thinking bigger: Addressing the relationship between structure and properties

While small changes may have some impact on students' understanding of IMFs, ultimately our larger concern is how students' understand these interactions in terms of the bigger picture of structure-property relationships. Much of the literature on students' understanding of the various concepts related to the connection between structure and properties has focused on identifying and diagnosing difficulties. Significantly less work has been done to address how we can improve student understanding of this core chemistry concept.

One possible solution could be the use of learning progressions to describe the progression of ideas and topics needed to achieve a thorough understanding of the structure-property relationship.^{47–49} While there has been much debate as to the definition of learning progressions, Duschl and colleagues have described them as "conjectural or hypothetical model pathways of learning over periods of time that have been empirically validated." Learning progressions should be grounded in theories of learning and cognition and should map students' progress to more sophisticated levels of knowledge.⁴⁸ Several researchers have noted that traditional chemistry curricula often sacrifice breadth for depth; that is, they emphasize a large number of individual concepts in a "laundry-list approach" rather than focusing on successfully integrating and connecting a small number of core ideas.^{47,50,51} Corcoran and colleagues stress

that learning progressions should draw upon research on students' understanding of the relevant concepts and how they learn to clearly define an appropriate sequence of topics needed to develop a deep understanding over time. Additionally, learning progressions should be tested for validity ("Does instruction based on the learning progression produce better results for most students?").⁴⁹ Learning progressions have already been developed for a variety of scientific topics including the nature of matter⁴⁷, scientific modeling⁵², energy⁵³, and chemical thinking⁵⁴. These progressions can be used to aid the structure of chemistry curricula, informing how core concepts are addressed through the course and the design of effective assessments to highlight improvements in student understanding.

Cooper and Klymkowsky have designed a general chemistry curriculum, Chemistry, Life, the Universe, and Everything (CLUE)^{51,55}, to address student difficulties, not only with the relationship between structure and properties, but with a wide array of foundational chemistry concepts. The curriculum continually revisits and emphasizes three core ideas, structure, properties, and energy, while also focusing on the interconnectivity of these ideas and the role of forces.⁵¹ The interplay of these concepts throughout the first semester of the course can be seen in Figure 3.2.



Figure 3.2: The connectivity of the CLUE curriculum's three core ideas throughout the first semester. Reprinted with permission from Cooper, M. M.; Klymkowsky, M. W. *J. Chem. Educ.* **2013**, *90*, 1116–1122.⁵¹ Copyright 2015 American Chemical Society.

Cooper and Klymkowsky designed the curriculum using a purposefully selected progression of topics that build off of each other and reflect the tenants of meaningful learning.⁵⁶ They have incorporated a learning progression for the structure-property relationship³, and have evidence to show students' improved understanding of the various topics involved. Specifically, students enrolled in the CLUE course experienced less difficulties constructing appropriate Lewis structures and were better able to identify of the chemical information encoded in these structures than their traditional curriculum counterparts.^{2,3,7} We will explore additional evidence of CLUE students' improved understanding of intermolecular forces in Chapter 7.

We know that students possess a wide range of alternative ideas and misunderstandings when it comes to intermolecular forces and the relationship between structure and properties. While much work has been done, there is certainly room for additional research into these ideas. The next chapter will outline our efforts to explore students' understanding of the connection between structure and properties through interviews. Previous work from our research group indicated that many students did not believe that physical and chemical properties could be determined from a Lewis structure.² We were interested to see if students could effectively use structures of various compounds to predict physical and chemical properties and, if not, then how did they determine the properties of a substance? REFERENCES

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CHAPTER IV: AN INVESTIGATION OF COLLEGE CHEMISTRY STUDENTS' UNDERSTANDING OF STRUCTURE-PROPERTY RELATIONSHIPS

Preface

This chapter discusses findings from our research into how students understand the relationship between structure and properties. This research has been previously published in the Journal of Research in Science Teaching and is reproduced here in full with permission from publisher John Wiley and Sons:

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Introduction

The relationship between the molecular-level structure of a substance and its properties is a core concept of chemistry and a vital skill for understanding a subject like organic chemistry. The foundational idea that the arrangement of atoms and electrons in a substance directly affects the macroscopic, observable properties of that substance is powerful and can provide students with a scaffold on which to build their understanding of a wide range of chemical phenomena. One of the major goals of effective chemistry instruction, therefore, must be to help students learn the knowledge and skills that will allow them to make the connection between molecular-level structure and macroscopic behaviors in a meaningful way. Without a robust understanding of the underlying ideas that allow the structure-property connection, there is no organizing framework for most of chemistry and students, out of necessity, resort to memorization and

generation of heuristics. Nowhere is this more true than in organic chemistry where literally hundreds of seemingly different reactions and interactions can be introduced within one course. If students are unable to use structural cues to determine how and why molecules interact, we cannot be surprised when organic chemistry is thought to be all about memorization.

Unfortunately, the road from structure to properties (and back) requires a long chain of inferences and the application of sets of rules that may appear to be unconnected to the goal at hand. We have previously reported that students have great difficulty with many of the tasks required along the road from structure to properties, including drawing structures themselves and using structures to predict both physical and chemical properties.^{1–3}

Our goal in the work discussed here was to delve more deeply into the ways in which college students use the molecular-level structure of a substance to predict its macroscopic properties. Before we can begin to address the difficulties that students clearly have, it is important to identify how these problems arise so that more effective curricula and pedagogical approaches may be developed.

Background – Misconceptions, conceptual change, and dual processing Misconceptions

Most educators would agree that the development of conceptual understanding is a major, yet somewhat elusive, goal of all science education. As the NRC committee on Discipline Based Science Education reports, "it is important to begin by identifying what students know, how their ideas align with normative scientific and engineering explanations and practices (i.e., expert knowledge), and how to change those ideas that are not aligned".⁴ Indeed conceptual understanding and identifying "misconceptions" (sometimes known as alternate conceptions, or

naïve ideas) that would hinder student understanding of chemical concepts is a major, active research area in chemistry education. While much of the work on conceptual understanding focuses on younger children^{5,6}, it is clear that college students also have a wide range of misconceptions.^{7–13} Indeed, over 120 papers on conceptual understanding in chemistry have been published in the last decade.⁴

In this research, we investigate college students' understanding about how structure affects physical properties. While this is a core concept of chemistry, it has not been the focus of many studies. For example, Smith & Nakhleh report that many college chemistry students retain the well-documented^{14,15} misconception that when a substance is melted, covalent bonds are broken (rather than intermolecular forces being overcome).¹⁶ The focus of their study was not the structure of the compounds but rather the process of melting or dissolution. To date, in fact, there has been little research about the origin of such ideas or how students' understanding of structure impacts their models of phases or phase changes.

While there are hundreds of different ideas that have been categorized as misconceptions, their origin and extent differ widely. Chi has proposed a tripartite classification of incorrect student beliefs, ranging from the level of a single idea to ideas that are robust, pervasive, and stem from multiple sources.¹⁷ Perhaps what is most relevant to chemistry instruction is that the deep underlying ideas of chemistry, upon which the rest of the subject is scaffolded, are rarely based on a single concept, idea, representation, or definition. Even a seemingly simple task requires students to organize and synthesize a huge amount of information. For example, the "misconceptions" that sodium chloride exists as molecules¹⁸ and that bond breaking releases energy^{19,20} are widely prevalent, but the sources of confusion are complex. A correct explanation of why sodium chloride does not form molecules or why bond breaking is endothermic, is

complex and would require an understanding of a range of ideas and a great deal of cognitive effort. Similarly, the focus of this paper, structure-property relationships, requires students to concatenate a sequence of inferences and apply several sets of rules before they can provide a meaningful prediction about structure-property relationships.

Conceptual change

While a misconception at the level of a single fact may be addressed by revising or rebuilding the idea itself, overcoming flawed mental models involves conceptual change. Mental models are students' internal representations of phenomena and, while they need not be accurate, they must be functional and modifiable. The effectiveness and detail of the user's mental models may be restricted by their previous experiences with a similar task, technical background, and how they think about the system.^{21–23} Constructing appropriate mental models is particularly important in chemistry since much of chemistry deals with scales that are not visible.

While much has been written about teaching for conceptual change, there are, in fact, no evidence-based, well-tested theories of conceptual change that are widely accepted.²⁴ Most researchers agree that students bring a collection of assumptions, ideas, and skills with them. The researchers differ, however, in that some interpret student ideas about concepts as fairly coherent (if naïve or mistaken) explanatory frameworks^{17,25}, while others support an approach in which students construct loosely woven explanations of phenomena from smaller fragments.^{26,27} As diSessa has pointed out, these different theories may necessitate quite different instructional approaches to enact conceptual change.²⁴

If students have a somewhat coherent (but incorrect) theory about a particular concept then it should be possible to establish conditions in which they can "reconstruct" that theory through

dialog and appropriate instruction.²⁸ In contrast, if students possess "knowledge in pieces" and construct explanations that are loosely woven, highly contextualized, and often composed "on the fly", then different instructional strategies may be needed. For example, Linn has proposed scaffolded knowledge integration frameworks that may promote more robust and coherent models.²⁹

Another possible approach to the development of coherent conceptual development involves learning progressions that explicitly develop difficult ideas in a way that allows students to integrate the fragments and ideas into a coherent whole are also proposed as a way to help students develop more robust and self-consistent conceptual frameworks.^{30–34} It may be the case that both approaches are valid in different situations. In either case, it is important to ascertain the knowledge and assumptions (both explicit and implicit) that students bring with them before any attempt to develop instructional materials designed to improve student understanding. With these ideas in mind, our initial goals were to elicit student ideas about the connection between structure and function, to investigate the origins of these ideas and to see how coherent they were. However, as the interviews progressed, we realized that another factor was emerging: instead of using the methods that they had been taught, to elicit structure-property connections, many students were using self-generated (personal) shortcuts or heuristics.

Heuristics and dual processing

Most of the earlier research and proponents of both approaches for promoting conceptual change have been focused on systems with macroscopically observable behavior that are often encountered in physics and physical science instruction or macroscopic biological systems. However, in subjects like chemistry that encompass not only the macroscopic level but also the

molecular-level, there is an additional level of abstraction since students are unable to directly observe phenomena and therefore must rely on increasingly complex representational systems to understand concepts, models, and ideas. Because of this abstraction, molecular-level understanding must depend on the representational system used and the students' ability to use it. The difficulty in navigating between molecular, symbolic and macroscopic domains has long been understood, but it is exacerbated as the representational systems that must be used to encode information increase in complexity.³⁵

Experienced chemists can look at a chemical structure and determine the shape, areas of high or low electron density, types of intermolecular forces (IMFs), acidic hydrogens, and reactive centers almost automatically. But beginning students, ideally, must go though a long sequence: 1. Construct an appropriate structure that contains enough information to make further inferences (typically taught using a set of rules) showing where all the bonds and non-bonding electrons are located, 2. Translate the two-dimensional structure to a three-dimensional structure (using another set of rules), 3. Use knowledge of relative electronegativities of atoms to predict bond polarities, 4. Use the three-dimensional structure and bond polarity information to make inferences about the overall polarity of the molecule, 5. Use this information to determine the types of IMFs that cause interactions between molecules, and 6. Use all this information to predict how molecules will interact.² So, while the concept that the molecular-level structure can be used to predict properties is central, its application is complex and difficult and we should not be surprised when students struggle, even after several years of college chemistry courses.

In fact, instructors have implemented a range of heuristics that are taught to students to help them construct molecular representations and use them to predict properties. For example, the "octet rule" allows students to construct Lewis structures without having to consider how or why

the representation should look this way. "Like dissolves like" allows prediction of what substances will be soluble in a given solvent. Such heuristics allow rapid decisions and predictions to be made without considering the ideas that allowed their development. While they are useful "rules of thumb", it is important to remember that they are not explanations for a particular phenomenon or concept.

There are only a few studies that have investigated the use and development of such heuristics in chemistry. Taber, for example, has reported on the problems arising from the use of the "octet" rule.^{11,36} In addition to heuristics that are explicitly taught in classroom contexts (instructionally derived), it has been shown that students also develop their own heuristics to help them simplify the reasoning that must be used to answer complex questions.^{37,38} Maeyer and Talanquer have reported on students' use of heuristics during ranking tasks such as those found on typical general chemistry examinations. Students' thinking was categorized as one of four heuristics: recognition, representativeness, one reason decision-making, or arbitrary trend. These researchers did not explicitly ask students to use the structure of the substance to make predictions and rankings, but rather asked them to discuss the criteria they used to make their decisions. In no case did the students' rankings rise above 20% correct, which may be attributed, in part, to the complexity of the task.³⁹

The extensive use of such heuristics has been explained by dual process theories of human cognition, which have been developed in a number of disciplines.⁴⁰ For example, Stanovich and West introduced the idea of System 1 and System 2 types of thinking, where System 1 thinking is rapid, automated, and requires less cognitive effort; it is the "default mode" for most processes.⁴¹ System 1 thinking is the source of the well-documented literature on cognitive biases and simple errors.⁴² Most people use System 1 the majority of the time: it allows for the
performance of multiple tasks simultaneously, and does not require a great deal of cognitive effort. On the other hand, System 2 thinking is sequential, deeper, and requires effort and attention, resulting in the thinker bearing down on the idea at hand and concentrating hard. One of the difficulties in learning science (or learning anything) is that it is almost always necessary to use System 2 thinking processes and to consciously over-ride System 1.

The use of heuristics or shortcuts allows us to use System 1, the default mode, when considering complex problems, and the heuristics we teach are designed to do just this. It is not surprising, therefore, in situations where an extensive chain of inference is required, such as relating molecular structure to properties, that students may also develop their own heuristics to answer questions rather than rely on their knowledge of scientific principles. While the use of heuristics becomes ever more necessary as the chemistry becomes more complex, and experienced chemists automatically default to them to lessen the cognitive load of a particular task, it is important to remember that they are not explanations. For example, the "octet rule" is very helpful when determining how to draw correct structures, however it tells us nothing about the reasons for bond formation. Similarly "like dissolves like" is a useful shortcut, but provides no insight into the molecular level processes, energy and entropy changes that are associated with the formation of a solution.

Purpose and significance of the study

In this study, we interviewed students from general and organic chemistry. We specifically asked how they would use the molecular-level structure to determine physical properties such as melting and boiling point. Our focus was on organic chemistry students since a robust understanding of the principles of organic chemistry is predicated on the idea that students can

predict how a substance will behave from an inspection of its molecular structure. We included general chemistry students because it is in general chemistry where these skills are first developed, and we wanted to see how (whether) these skills change over time.

Our goals were to better understand the process by which students determined properties such as relative melting or boiling points from a structure and what factors they took into consideration (i.e. molecular geometry or polarity). While other studies have looked at student reasoning about relative phase change temperatures or solubilities^{16,39}, none have explicitly probed students' understanding of how and why the structure determines these properties. Therefore, we decided to use simple structures so that we did not overwhelm the students. For example, while some common substances like fats and sugars may be familiar to students, their structures may be too complex for a novice to analyze. We believe this study is important because it probes a fundamental construct of chemistry that **all** students should have mastered by the time they finish general chemistry. In most general chemistry courses (and certainly the courses that these students were enrolled in) the topics covered by our interviews make up about 25% (five chapters out of 20 chapters that are taught), and approximately 50% of the material in a first semester general chemistry course. Indeed, by the time students reach organic chemistry most instructors spend little time on the development of these skills because they are such an integral part of the prior knowledge that is expected. While most organic chemistry textbooks do briefly review structure property relationships in the first chapter, the majority of the course is taken up with more advanced concepts that build on these ideas. For example, how molecules interact to produce new products, how changes in molecular structure and interactions are related to energy changes, and how the three-dimensional structure can be represented and understood in

two-dimensional drawings. All of these ideas and skills are predicated upon the kind of understanding that we were probing in this study.

This study is part of a larger series of studies in which we have used a variety of methods to investigate student understanding of molecular structure and properties. In our earlier studies, we investigated whether students were able to draw and use chemical structures to make predictions about properties.^{1–3} The study on which we report here aims to elucidate why students have such trouble with this concept. Using a basic, qualitative research design, a semi-structured interview protocol was implemented to further investigate students' ideas about structure-property relationships. Taken together, these studies consist of a mixed-methods sequential explanatory study.⁴³

Our study focused on two research questions:

- RQ 1: Do students use molecular-level structures to make predictions about the macroscopic properties of a substance, and if so how?
- RQ 2: How do students enrolled in general and organic chemistry use representations of chemical structures to make predictions about macroscopic properties of substances?

Methods

Setting and participants

This study was conducted at a public southeastern research university of about 20,000 students. At this university, general chemistry and organic chemistry are taught in lecture sections of between 100 and 150 students. Approximately 1500 students enroll in general chemistry per semester and 600 in organic chemistry. Participants were volunteers who were

solicited by email from second-semester general chemistry students (GC2, N = 7), first-semester organic chemistry students (OC1, N = 5), and second-semester organic chemistry students (OC2, N = 5). In order to participate, students must have completed at least one semester of general chemistry; this was to prevent undue confusion for students who had not yet been exposed to topics relevant to understanding the relationship of structure and property such as polarity and intermolecular forces. All of these students signed informed consent forms.

Of the 17 participants, 5 were male and 12 were female; 11 participants pursued biologyrelated majors, 3 were chemistry majors, and 3 were engineering majors. All participants received either an A or a B in prior chemistry coursework. All of the students were enrolled in chemistry courses that either "covered" the material (general chemistry) or depended on students knowing these ideas (organic chemistry). The students came from different courses taught by different instructors, using different pedagogies. In general, most students in these courses completed on-line homework assessments and in class written quizzes where they would write or draw a response, often after group discussion. In general chemistry, all the course examinations were multiple choice, but in organic chemistry typically about half the examination was composed of student constructed responses. All students in these courses took final examinations in the form of American Chemical Society normalized examinations⁴⁴ and, on average, scored above the national norm. It is important to state here that these are students who have done everything that is asked of them, and who appear to have a firm command of the material when traditional assessments are used. What follows is in no way intended to imply that the problems we uncover lie with the students. As we will discuss later, we believe it is the structure of the curriculum and the accompanying assessments that do not provide an appropriate learning environment in which students can be expected to develop these complex ideas.

Interview protocol

The semi-structured interview protocol began by asking students what kinds of tests they might use in a chemistry laboratory to identify a substance. This was to help students recall chemical and physical properties with which they might be familiar. If students did not spontaneously respond with melting point or boiling point tests, the interviewer suggested that such properties were measurable in the laboratory. Students were then asked specifically, in reference to water, ammonia, and ethane, about the types of properties the compound might exhibit. These were compounds that were (or should have been) familiar to the students. The interviewee was then asked to construct a Lewis structure or other structural representation for these compounds and asked how they might use that structure to help them explain the properties (particularly melting point or boiling point) of that compound.

The second portion of the interview was designed to reflect the types of questions the students would typically experience in their chemistry course. Students were given several pairs of compounds and asked to pick, for each pair, the compound that would have the higher boiling point and explain why. Table 4.1 lists each of the pairs given and the reason why they were chosen. The table also includes reasoning that we would expect a student to use when explaining why one compound would have a higher boiling point than the other. The compounds chosen for discussion were simple structures containing no more than two carbon atoms. It should be noted that if students had difficulty constructing any of these structures throughout the protocol, the interviewer would provide the student with structural cues such as clarifying dimethyl ether as CH₃OCH₃. Additional methods outlining the full interview protocol are available in Appendix B.

Table 4.1: Pairs of compounds presented to students, the reasons for choosing this comparison, and the expected student reasoning

Pairs of compounds	Reason for our choice	Expected student reasoning	
CH ₃ CH ₃ and CH ₃ CH ₂ OH		Ethanol has a higher boiling/melting point	
	Different molecular weights, different	because it has stronger intermolecular forces	
		(specifically hydrogen bonding and dipole-	
	types of IMFs	dipole), which require more energy to overcome	
		during a phase change.	
CH3OH and CH3CH2OH	Different molecular weights, same types of IMFs	Ethanol has a higher boiling/melting point	
		because it has stronger London dispersion forces,	
		which require more energy to overcome during a	
		phase change.	
CH ₃ CH ₂ OH and CH ₃ OCH ₃	Structural isomers,	Ethanol has a higher boiling/melting point	
	same molecular	because it has stronger intermolecular forces	
	weights, different	(specifically hydrogen bonding), which require	
	types of IMFs	more energy to overcome during a phase change.	

Data collection

A post-doctoral researcher conducted the first five interviews and was then joined by a graduate student. After co-conducting four interviews, the remaining eight interviews were conducted by the graduate student (the second author on this paper). The length of the interviews varied from 30 to 60 min depending on the amount of information that the students provided. For the interviews, audio and student-constructed representations were collected using a *LiveScribe* pen, which can replay both the audio and student drawings in real-time.⁴⁵ Audio was also recorded using a digital voice recorder.

Data analysis

After the interviews were conducted, a post-doctoral researcher, an undergraduate research assistant, and a graduate student transcribed them verbatim. Using a qualitative approach based on grounded theory techniques, a graduate student, a post-doctoral researcher, and a faculty member analyzed the interview transcripts and *LiveScribe* data for emergent themes and

commonalities using open coding.⁴⁶ Initial codes were created and revised via constant comparison.⁴⁷ Multiple revisions were required in order to address the complex nature of student knowledge of the structure-function relationship. After several iterations of coding, four overarching themes were identified that encompassed the major issues experienced by students in their explanations of this relationship. Although these themes stemmed from widely differing sources, each was identified as contributing to student difficulties and emerged during the reasoning tasks. These themes are: 1) inappropriate models of phases/phase change, 2) representational difficulties, 3) language and terminology issues, and 4) use of heuristics in student reasoning (whether appropriate or not). Each of these themes in student difficulties consists of a number of subcategories that we collapsed together to produce the major concept.

Findings

Emergent themes in students' difficulties in reasoning structure-property relationships

In response to our first research question (RQ 1), we present examples of each overarching theme that emerged from the interviews and then illustrate how these themes combined and were used by students to make predictions about melting and boiling points of various substances. Table 4.2 presents each student's pseudonym, their level of chemistry, and which of the four main over-arching themes were present for their reasoning.

Table 4.2: Students' pseudonyms, chemistry course, and themes that arose during their interview. A count is shown for a specific category if the student showed at least one instance of the code during their interview.

Pseudonym	Course	Phase/ Phase Change	Represen- tations	Terminology	Heuristics		
					Personal	Instruc- tional	More Means More
Noah	GC2	1	0	1	1	1	1
Brittany	GC2	1	0	1	0	1	1
Tina	GC2	1	1	1	1	1	0
Susan	GC2	0	0	1	1	0	0
Erin	GC2	0	1	0	0	1	0
Lucy	GC2	0	1	1	1	1	0
Justin	GC2	0	1	0	1	0	1
Robin	OC1	0	1	0	1	1	1
Ted	OC1	0	0	1	1	1	1
Lily	OC1	1	1	1	1	1	1
Marshall	OC1	1	0	1	1	0	1
Victoria	OC1	0	0	1	0	0	1
Daisy	OC2	1	0	1	1	0	1
Joy	OC2	0	1	1	1	1	1
Jill	OC2	1	1	1	1	0	1
Jane	OC2	1	0	1	1	0	1
Joe	OC2	1	1	1	0	1	1

Models of phases or phase change

Eight of our interviewees did not possess a coherent model of the structure of solid, liquid, and gaseous simple molecular compounds, which typically emerged when students were asked to draw structures representing different phases.

Joe (OC2) struggled with drawing a molecular-level depiction of a solid. He seemed concerned about the idea that ethane might form a solid because, if ethane did form a solid, this would require the molecules to be bonded together rather than interacting. "I would say they, if you're saying there is a solid, I guess they would have to bond…because they're just so compact". He attempted to draw his idea of what bonded ethane would look like in the solid

phase, with molecules bonded together, as seen in Figure 4.1(a).



Figure 4.1: (a) Joe's depiction of solid ethane, (b) Jill's depiction of solid ethane, and Brittany's representation of (c) water going from the solid phase to the liquid phase and (d) water going from the liquid phase to the gaseous phase

Similarly, Jill (OC2), experienced difficulties depicting solids and liquids on the molecularlevel. Her representations of solids and liquids appear to show that they are covalently bonded in a network structure rather than held together via intermolecular forces. Jill was quite consistent with her depictions of solids as networks, as seen in Figure 4.1(b) with solid ethane, using the same idea for water, ammonia, and dimethyl ether.

While Jill and Joe experienced difficulties explaining their model of phases, Brittany (GC2) struggled to explain the process of a phase change. When asked explicitly to describe the process of ice melting on the molecular-level, she responded, "Hold on, I've never thought about all this stuff before". Brittany (GC2) stated that the "bonds" between the molecules would break, which would leave behind individual water molecules. "Umm I guess it's, I guess maybe the bonds are

stronger in a solid and they're weaker in a liquid so it's like, so it's like move, like water like moves and ice doesn't. So it's like movable I guess. Malleable".

It is well documented that students often confuse intermolecular forces with covalent bonds^{14,48,49}, and it is entirely possible that Brittany was confused about the difference between intermolecular forces and covalent bonds, but her structural representations of water in the solid and liquid state still contain water molecules. As she discussed the transition to a gas, however, Brittany broke the covalent bonds within the water molecules; she drew structures for us that clarified what she meant, clearly showing interactions between molecules breaking from solid to liquid and H–O covalent bonds breaking from liquid to gas as seen in Figure 4.1(c) and (d).

Each of these students struggled with their understanding of either phase or phase changes. They each provided different representations in an attempt to explain their model, but in doing so, they became aware that something was wrong. Their inability to construct appropriate representations and extract meaning from them severely hindered their understanding. If students cannot provide an appropriate representation for each phase, it is unlikely that they will be able to make predictions about relative phase change temperatures or the factors that affect phase changes.

Use of representations

Nine participants experienced some form of representational difficulty during their interview, although not all were directly related to phase or phase changes. Looking back at Jill's network model of solid ethane in Figure 4.1(b), it is understandable that she explained the process of boiling in terms of bond breaking since her representations made no reference to intermolecular forces. She indicated in her interview that, as a solid melted, some of the bonds

were broken. Then, as the substance moved into the gas phase, the individual molecules separated. Her difficulty with this concept was apparent, since there were numerous false starts in her attempt to explain the bonds that break during the boiling process of dimethyl ether:

Like if you broke this (C-H bond in Figure 4.2(a)) you'd have two dimethyl ethers versus (Figure 4.2(b)) one dimethyl ether and one anhydrous, or one with a partial negative charge on each carbon. I don't know, I can't, I don't know which way is right on that. I suppose that I've never really thought about...this makes, this sounds better (pointing to Figure 4.2(b)).



Figure 4.2: (a) and (b) Jill's first and second attempts at depicting dimethyl ether transitioning from a solid to a liquid and (c) Lucy's representation of nonpolar dimethyl ether

Her first approach, Figure 4.2(a), is consistent with the lattice form she drew for previous compounds in the interview. With this representation, she realizes that, by breaking bonds during the boiling phase change, she would have resulting dimethyl ether molecules missing hydrogens.

In her second approach, Jill redraws her lattice structures, connecting dimethyl ethers with covalent bonds between the hydrogens. While this solves the problem of losing hydrogens in the boiling process, she voices concern that now each hydrogen would have two bonds and hydrogen "like it's only got the one electron, one you know so it can only technically bond to one thing". It is important to note that she refers to the tendency for hydrogen to only form one bond as the rule of hydrogen bonding (a possible terminology issue). She understood that network structures did not make sense for her solids, but, as she stated, "umm I haven't really thought about that" despite the fact that she is in her fourth semester of college level chemistry.

A subtler problem emerged from Lucy (GC2), who knew that the strength of the IMFs determines boiling points. Her problem, however, originated with her difficulties in translating the two-dimensional Lewis structure into a three-dimensional shape. Since she drew dimethyl ether as linear (Figure 4.2(c)), she believed that it was non-polar because the bond polarities cancelled:

So if you were gonna kind of split this up, oxygen obviously has the slight negative charge and carbon's gonna have like a slight positive charge but if this is going this, umm opposite ways, it goes towards the negative and then if this is going (drawing) towards the negative then these two arrows cancel each other out.

In fact, only three of the students, all of whom were in general chemistry, used bond polarity vectors to determine molecular polarity and the resultant types of IMFs.

Language and terminology

It has been well documented that students often struggle with the use of scientific language in their chemistry courses.⁵⁰ Some of this difficulty stems from the use of words that have not only

a specific meaning in chemistry, but also a more colloquial use. For example, students may say that a reaction has come to equilibrium but not understand that the process is still ongoing or that the use of the term volatile, commonly meaning explosive or unstable, is used in science to indicate a substance that is easily vaporized.

Most of the participants (14 out of 17) experienced some form of terminology and language problems. During our interviews, it became clear that many were confused about the meaning of words that describe interactions such as bonds, intramolecular forces, and intermolecular forces (such as hydrogen bonding, dipole-dipole, and London dispersion forces). Jane (OC2) was aware that these terms are easily confused:

Umm hydrogen bonding is between if, is it intermolecular force? I always get confused if it's inter or intra because they're two different things but it's between two molecules and it's umm, my professors always do like the little dotted line that shows like the attractions.

That is, Jane, while not sure of the name for intermolecular forces, did understand that these interactions are between two molecules.

Joy (OC2), on the other hand, illustrated hydrogen bonding as both within and between molecules while drawing her structure for ammonia.

Interviewer: Ok. So could you just show me how it hydrogen bonds? *Joy*: Oh it's right there between the H and the N. Yeah. I don't know how I just... *Interviewer*: So if you had another ammonia molecule could you draw another one for me?

Joy: (drawing additional ammonia with dashed line between the molecules) *Interviewer*: Ok so umm what would this be? Like that, you just drew dotted?

Joy: Oh this is a hydrogen bond.

Interviewer: Ok. And you said that this (indicating the N-H bond) is also a hydrogen bond?

Joy: Yeah.

Her depiction of hydrogen bonding, seen in Figure 4.3, showed both an interaction between the nitrogen of one ammonia molecule and the hydrogen of another as well as the N-H bond within one molecule (indicated by positive and negative charges). Joy's confusion about the term hydrogen bonding is understandable, since, typically, the term bond is used between two atoms in a molecule. At the same time, she also remembered hydrogen bonding as existing between two molecules. To compromise these two ideas, she decided that it could be both.



Figure 4.3: Joy's depiction of hydrogen bonding in ammonia, both within a molecule and between two molecules

Unfortunately, the idea that intermolecular forces are what most textbooks refer to as covalent bonds was quite pervasive. Ted (OC1) also struggled with this idea. At the beginning of his interview, Ted referred to hydrogen bonding as the bond between oxygen and hydrogen within the water molecule rather than an interaction between two water molecules. This became a significant terminology problem that followed him throughout his interview as seen when he later compared the relative boiling points of ethanol and ethane:

Umm well you know this one's (ethanol's) going to have the higher boiling point because it's got a strong, the hydrogen bond that's in it right here is going to be a lot stronger to break. So, I mean its going to be more difficult to break since it's a lot stronger bond so you automatically have higher, a higher boiling point than this (ethane).

After further questioning from the interviewer about what specifically breaks when a substance boils, Ted realized there was an inconsistency in his prior reasoning and the bonds within a molecule should not be breaking. He then proceeded to describe an attractive force present between the molecules, but, since he had already allocated the term hydrogen bonding to the O-H bond, he called this force a Van der Waals interaction:

I'm guessing there is not a bond between these two (ethanol's) but there is like a little bit of maybe, not even London dispersion, but there's like an attraction since this is a partial negative side of the polar and this is the partial positive...I don't even know why I am thinking like London dispersion cause that's like within the molecule I want to say or maybe it's, hold on, let me umm...Van der Waals interactions.

While Ted correctly identified that there are attractive forces between two ethanol molecules and had an understanding of the underlying concept of intermolecular forces, his difficulties with terminology created challenges for him in communicating this knowledge. Presumably, this terminology issue could also create problems in making sense of lectures, notes, and textbook

content. It should be noted that he described hydrogen bonds and London dispersion forces as within-molecule interactions and Van der Waals forces as between-molecules interactions.

These examples of student difficulties related to representing and communicating phases and phase changes were not unique to the students discussed here. Sometimes the students' issues with phases occurred in combination with their difficulties in producing appropriate representations or terminology issues. Each of these problematic areas combined with others in slightly different ways, making each student's response unique.

Use of heuristics in student reasoning

In the second half of the interviews, students were given the three prediction tasks shown in Table 4.1 and were asked to explain their reasoning. We anticipated that students would construct structures, use them to predict the types and strengths of intermolecular forces present, and then use this information to predict which compound would take more energy to separate the molecules, which they would relate to the boiling or melting point. What emerged for all students, on at least one occasion, was a heuristic that had either been instructionally derived or personal. Interestingly almost all of the heuristics used some version of what may be akin to diSessa and Hammer's "more means more" p-prim^{51,52}, that is, they almost all involved counting something, be it oxygens, carbons, hydrogens, bonds or intermolecular forces, and used these surface level characteristics to predict properties. While some of these heuristics lead to a correct prediction, many of them did not and several were complicated by problems with representations and language that we have already discussed.

Heuristics – Instructionally derived

Victoria (OC1) is an example of one student who used a heuristic that she had been taught for reasoning about the differences in boiling points of ethanol and dimethyl ether. She discussed how the presence of oxygen is important to compare the boiling points:

Yeah because they both have one oxygen in them...I was always taught that if there was an oxygen in there the boiling point is going to be higher...than if there wasn't an oxygen and if it was an alcohol it would be higher than ether because of the hydrogen bonding.

In this instance, Victoria relied on sets of heuristics to rationalize the difference in boiling points. While she arrived at a correct conclusion, she did not explain the differences in terms of intermolecular forces. Her reasoning is surface-level, as with many other students, in that it focused only on the elements and functional groups present, but it did bring her to the correct conclusion.

Heuristics – Personal

Interestingly, more students (N = 10) used a personal heuristic in comparison to an instructionally derived heuristic (N = 7). For example, Joy (OC2) developed a similar heuristic to Victoria that relied on the presence of oxygen in organic compounds to determine the relative boiling point. Unlike Victoria, however, Joy's version of this heuristic indicated a *lower* boiling point when oxygen is present. "I wanna say this one (ethanol) has an O, a hydroxyl group on it so I feel like it would boil quicker than the hydrocarbon". While she never explained her reasoning for this relationship, she later changed her explanation (and her prediction) to include hydrogen bonding when asked to draw out the Lewis structure (including drawing out the O–H

group) for ethanol. When questioned about why she changed her reasoning, she replied "Well I wasn't really thinking about it then. I just looked". In this situation, Joy was even aware herself that she defaulted to a System 1 level thinking and that only after further prompting did she take it a step further to discuss hydrogen bonding.

A few students used a phenomenological approach, indicating that heavier molecules would have a higher boiling point because heavy molecules would be harder to get into the gas phase. Justin (GC2) invoked an instructionally derived "more means more" heuristic when he compared the boiling point of methanol and ethanol. "I think it's [ethanol] a bigger molecule so it, every property increases except for viscosity. That's what, that's what I memorized at least". Robin (OC1), however, used a personal variant of this "more means more" reasoning: "So it's (methanol) a much smaller molecule first off and it's a lighter molecule…so it will be umm it will go to the gaseous state more readily so it will have a lower boiling point". Robin's ideas may stem from an inappropriate application of gravitational effects, which are negligible at the molecular scale, or may simply be another p-prim – heavier things are hard to move.⁵³ Robin was incorrect in her predictions for ethanol and dimethyl ether, presumably because her heuristic was not useful for molecules with the same molecular weight.

In a number of cases, the representational or language issues that led to difficulties with student models of phases were also folded into the reasoning that students used to support their heuristics. For example, some explanations were predicated on a model in which covalent bonds must be broken to change phase. Joe (OC2) used a "more means more" heuristic to explain that the number of bonds within a molecule directly affected the boiling point: "This carbon (ethanol) is more substituted so I would say this carbon (methanol) has a lower boiling point...it has less bonds to break". Here, Joe indicated that ethanol had more bonds, which he believed would be

broken as the ethanol was vaporized. Thus, his understanding seemed to be that ethanol had a higher boiling point because more bonds require more energy to break.

Jane (OC2) also used a similar personal "more means more" heuristic to compare the boiling points of ammonia and water, but she used the number of hydrogen bonds as part of her reasoning. "Because it [ammonia] has more, more bonds...The nitrogen has attached to three hydrogens but the oxygen's only attached to two...More bonds means more intermolecular forces so it should be, it should have a higher melting point". Jane (as discussed earlier) used the number of hydrogen bonds to predict that ammonia has a higher melting point than water. Her reasoning still involved breaking bonds during a phase change (which she called intermolecular forces). Additional examples for all themes are available in Appendix C.

Comparing general and organic chemistry students' reasoning of structure-property relationships

In reference to our second research question (RQ 2), it is clear that organic students performed no better than general chemistry students on these tasks, as seen in Table 4.2, despite their extra semester or two of chemistry. While this may be understandable, since instruction in organic courses typically does not dwell on material that students have presumably mastered in earlier courses, it means that organic students do not have a stable foundation on which to build their new knowledge. The major difference we found between the general chemistry and organic chemistry students was that the organic chemistry students' explanations were often **more** convoluted because they brought extraneous information to their discussions. For example, while comparing the relative boiling points of methanol and ethanol, Jill (OC2) originally determined that ethanol had the higher boiling point but then changed her mind:

Jill: ...I retract my previous statement. I think methanol maybe has a higher boiling point because this one's got more like steric hindrance like between the hydrogen bonds because the molecule's bigger so it's gonna be easier to break. *Interviewer*: Ok. How would you break it? What do you mean when you say break?

Jill: Like when you add heat to it or something it's gonna split up the, like all the bonds like if you were you're in a liquid phase you've got all these bonds here that are kind of crammed together and if you heat it up it's gonna start splitting all these bonds apart. You're gonna lose, lose water I guess.

Jill stated that "steric hindrance", depicted in Figure 4.4(a), caused ethanol to be less stable than methanol. It is unclear whether she was confusing steric hindrance with steric strain, but she believed that when these substances boiled, bonds were broken. She again invoked steric hindrance to correctly predict that ethanol would have a higher boiling point than dimethyl ether:

'Cause these bonds are gonna be stronger than a carbon, carbon like these two bonds (C—O and O—H bonds) are gonna be stronger than a carbon—hydrogen bond and then this one (dimethyl ether) has got uhh, even more steric hindrance than that one (ethanol) so these bonds are going to break easier.

Jill offered up yet another organic chemistry idea to explain why ethanol would have a higher boiling point than ethane:

Because alcohols, the alcohol group is a poor leaving group so it's, the bond's not going to be broken as easily. You'd have to protonate it first and turn it into water and then make it a leaving group. I think...Like the carbon—oxygen bond would be umm more difficult to break than a carbon—hydrogen bond.



Figure 4.4: (a) Jill's representation of the steric strain in a molecule of ethanol and (b) Lily's depiction of hydrogen bonding between two water molecules indicated by the arrows showing an electron pair leaving and a hydrogen attaching

For her explanation, Jill continued to discuss the idea of bond breaking when ethanol and ethane underwent the boiling process. Instead of explaining in terms of steric hindrance, however, she used the idea that -OH (alcohol) groups are poor leaving groups and, as a result, would make the carbon-oxygen bond harder to break. Here we have a confluence of a problematic model of phase change involving bond breaking combined with extraneous knowledge and a lack of distinction between a chemical reaction and a phase change.

Although Jill clearly has many problems, Lily (OC1) was the only student interviewed who exhibited at least one instance of every theme outlined in Table 4.2. When asked about water and how two water molecules would interact:

It would...umm...so yeah...this being the oxygen being the partially negative and the hydrogen being the partially positive like this bond right here (electron pair bonded to the oxygen) is going to break so that this proton (hydrogen on the interacting water) can come in and so like they are going to bond like that.

It quickly became apparent that Lily saw hydrogen bonding as a reaction in which the electron pair on the oxygen would leave so that the hydrogen on another water could come in and form a hydrogen bond, as seen in Figure 4.4(b). She had stated earlier in the interview that

hydrogen bonding was a bond within the molecule so her confusion is understandable. Inspection of her drawing showed that Lily was using the arrow notation learned in organic chemistry to mean two different things (neither of which was correct). The top arrow showed the electron pair "leaving" and the bottom arrow showed the hydrogen moving to take its place. It was here that her confusion about the notation used in organic chemistry became apparent. This problem then led to her unique explanation of what happens to water as it changes phase from liquid to gas:

Interviewer: Why would it (water) have a high boiling point?

Student: Because it takes a lot of energy to break the strong hydrogen bond hold. *Interviewer*: So which, can you just point to on the paper which bond you would be breaking?

Student: Umm you're going to be breaking the bond between these electron pairs so that they can go and that these protons can come in.

Daisy (OC2) used the concept of stability of different types of carbons for her reasoning that ethanol had a higher melting point than methanol: "there's two carbons here they help stabilize each other so it, and over-, and all it has, it's a more stable molecule versus the methanol". When prompted by the interviewer to explain, Daisy elaborated: "Umm well you typically think of it as the more the carbons the more stable in a way". It became clearer that she did not think the bonds were breaking, but that carbon-carbon bonds stabilized the molecule somehow, so that it took more energy to boil. She linked this stabilization to what she had learned about stabilization of carbocations in organic chemistry. "This is a primary carbon so it has at least one carbon attached to it. And I know that as you increase that like methyl, primary, secondary, tertiary your stability increases."

Discussion

As Table 4.2 shows, none of the students provided a completely coherent view of how to predict properties from structures. Interestingly though, most students were able to correctly predict which of each pair would have the highest melting or boiling point as shown in Table 4.3, even though they used some rather surprising reasoning strategies.

	ew proiocoi			
Pseudonym	Ethanol vs. Ethane	Ethanol vs. Methanol	Ethanol vs. Dimethyl ether	
Noah	Ethanol	Similar	Ethanol	
Brittany	Ethanol	Ethanol	Ethanol	
Tina	Ethanol	Not sure	Dimethyl ether	
Susan	Ethanol	Methanol (but almost the same)	Ethanol	
Erin	Ethanol	Ethanol (but almost the same)	Ethanol	
Lucy	Ethanol	Ethanol	Ethanol	
Justin	Ethanol	Ethanol	Ethanol	
Robin	Ethanol	Ethanol	Dimethyl ether	
Ted	Ethanol	Ethanol	Ethanol	
Lily	Ethanol	Ethanol	Dimethyl ether	
Marshall	Ethanol	Ethanol	First dimethyl ether, then ethanol	
Victoria	Ethanol	Ethanol	Ethanol (but almost the same)	
Daisy	Ethanol	Ethanol	Dimethyl ether	
Joy	First ethane, then ethanol	Ethanol	Dimethyl ether	
Jill	Ethanol	First ethanol, then methanol	Ethanol	
Jane	Ethanol	Ethanol	Dimethyl ether	
Joe	Ethanol	Ethanol	Dimethyl ether	

Table 4.3: Student prediction for highest boiling point in each comparison from the second half of the interview protocol

The only pair of compounds that more than two students predicted incorrectly was ethanol and dimethyl ether, presumably because the very common heuristic "more means more" was not applicable. Therefore, students were forced to move to explanations involving IMFs (typically hydrogen bonding) to provide a reason. When intermolecular forces were discussed, terms like hydrogen bonding and London dispersion forces were often used incorrectly. Even students who seemed to have a robust understanding of structure-property relationships had some discrepancies in their reasoning process. Erin (GC2, a bio engineering major) was one of the most articulate and accomplished students; she was able to correctly predict most of the properties of a compound by considering polarity and intermolecular forces. Interestingly, she used her prior knowledge in biology to reason through less familiar topics. For example, she provided a spontaneous (and quite sophisticated) discussion of London dispersion forces using a phospholipid bilayer (Figure 4.5) as an example:

It's a phospholipid bilayer...So what happens with the tails is umm at certain points of time, which is not very often but it does occur, that uhh by chance the electrons line up on one side just because they're constantly moving around and then that creates a very slight negative charge and that influences this one. So then that causes the electrons to be repelled and it causes a slight positive charge and so you have these moments when umm they're attracted because of partial negative and partial positive. But they only occur a very few time periods.

Even though Erin had a robust understanding of IMFs, she was not clear about the relationship between polarity and shape. Rather than the shape of the molecule influencing its polarity, she reasoned that the opposite is true. When discussing water's polarity and shape, she mentioned that "the shape is more characteristic of the fact that it's polar...it's because, that it's polar that it makes that shape (bent)". This caused her problems when later reasoning about dimethyl ether since she thought it was nonpolar, thus making it linear.



Figure 4.5: Erin's depiction of London dispersion forces in the phospholipid bilayer

From our interviews, with students who have been successful in their chemistry courses, it is clear that most have significant issues that impede their understanding of the relationship between structure and properties and that the situation does not appear to improve for students who have taken organic chemistry. Despite being specifically asked how they determine the properties of a substance from its structure, few students were able to extend their ideas to predicting and almost invariably invoked a heuristic. It was striking that, even though some students used heuristics that appeared to be very similar on the surface (for example "more means more"), they came to quite different conclusions using the same ideas.

Conclusions

What emerged from our interviews was a diverse tapestry of student thinking. Some students based their predictions on one overarching idea (more means more), some wove their model together from disparate facts and ideas, some students were hindered by their inability to construct and use structural representations, and some were hindered by language – either

misremembered or misunderstood. Each student constructed a different set of explanations and even those who had one overarching theme used it differently to come to different conclusions.

The major findings of this study are:

- 1. Each student individually constructed a different approach to the task posed. These approaches were hindered by other factors that interacted with each other in different ways.
- 2. Even students who used what appeared to be a similar approach (e.g. "more means more") came to different conclusions, using reasoning strategies and heuristics that emerged during the course of the interview.
- 3. Students in organic or higher-level courses seemed no more able to make the structure-property connection even though some students could answer questions correctly without consciously reasoning through the process.
- 4. Organic students sometimes used their extra knowledge inappropriately, for example, citing "steric hindrance" as a cause of differences in phase change temperatures.

What seems clear is that, as we move forward, simply categorizing "misconceptions" is not enough. The ideas and reasoning that students constructed were a result of the interactions between their understanding of what words mean, what structures mean, their models of how phase changes occur, and their willingness and ability to delve deeply into the underlying concepts. As Kahneman has written, "the automatic operations of System 1 generate surprisingly complex patterns of ideas, but only the slower System 2 can construct thoughts in an orderly series of steps".⁵⁴ Much of what the students had to say was not self-consistent and a number of students, on reflection or in response to a later prompt, changed their answer to a more scientifically reasonable one (see Table 4.3). Most students seemed to be relying on System I type thinking, rather than going back to first principles.

What became clear was that there was no single approach to solving this task and that the problems that arose in the students' explanations combined in different ways to produce varied results. Some students (especially those who used personal heuristics) appeared to use reasoning that they could apply fairly consistently (if not correctly), but students who used a similar overarching heuristic often came to different conclusions. It may be that a few of these students' reasoning strategies might more closely align with the "theory" school of conceptual change. While their reasoning might be consistent, it was often based on a flawed model of phase change or an inability to decode the meaning of structural representations and technical terms. However, we believe that most students' ideas were fragmented and inconsistent, students often changed their responses during the course of the interview in a process more reflective of the conceptual change theories of diSessa where students' responses are constructed on the fly from a loosely woven tapestry of facts, skills, and concepts.²⁶ What seems apparent from our findings is that, even after two years of chemistry courses, we have failed to help students make the crucial link between molecular-level structure and properties.

Questions and implications for teaching

This study seems to imply that students can take, and do well in, a "rigorous" set of chemistry courses without a thorough understanding of a core chemistry concept. All of these students were students who made good grades and yet many reported that they had never thought about the questions asked in our interviews. That is, students appear to be quite accomplished

and yet can harbor a range of problematic ideas that do not emerge under "normal conditions". It should be reiterated here that all the students in this study had already been taught this information and passed examinations, including those developed by the chemistry community (ACS examinations) that are designed to encompass what students should know at the end of a given course. This problem brings up two major questions:

When are heuristics "good enough"? By necessity, the use of reasoning shortcuts increases as students move through the curriculum. Clearly students in organic chemistry cannot be expected to laboriously draw out each molecule and go through the long, drawn-out process of determining the 3-dimensional structure, polarity, and types of IMFs for each question they are asked. Eventually, students must be able to "chunk" this material to avoid working memory overload, since they are also learning new material. However, if the answer to a question is "the boiling point is higher because of hydrogen bonding", we must be certain that students mean hydrogen bonding between molecules, rather than within molecules. That is, reasoning shortcuts or heuristics must be based on a firm foundation, otherwise what appear to be reasonable answers to questions may hide fundamental problems.

What can be done to improve student understanding in chemistry so that when students do use shortcuts, they are appropriate and useful? Our findings make it clear that there is something wrong with our conventional approach to the development of these complex ideas. Each student constructed a unique approach to predicting structure-property relationships that emerged from the interaction of the factors discussed above. Although we found misconceptions that had previously been well-documented, the ways in which these ideas played out in the context of the question prompts were different and it is clear that addressing each problematic area separately will not be helpful for students in developing coherent conceptual frameworks. Our findings

suggest that a scaffolded approach to the development of structure-property relationships, the development of progressions in which students are explicitly asked to connect their prior knowledge to new knowledge, and the explanation of how that knowledge will be used may help. For example, we have shown that students in a course designed in this way have an improved understanding of structure-property relationships and further studies are being conducted to assess how long these improvements are retained.^{3,20}

What is also clear is that, as students go through organic chemistry, they tend to lose sight of the underlying principles that determine how substances interact. That is, while they have more content knowledge than students in general chemistry, they may be no more able to apply basic principles and, in some cases, the extra knowledge may actually impede their understanding. In addition to reconsidering how structure-property relationships are taught in general chemistry, we also recommend that the teaching of organic chemistry begin with a thorough, lengthy review of structure, interactions, and properties. While most organic texts begin this way, in our experience many instructors assume that an understanding of intermolecular forces and (for example) simple acid-base chemistry are prior knowledge and all that is needed is a brief reminder. Unfortunately, this is not the case. In general, students do not begin organic chemistry with a robust understanding of these ideas and therefore are doomed to "play catch-up". Some students never do catch up and though they may emerge from the course with a database of memorized reactions, they are telling the truth when they inform the next generation of students that organic chemistry is all memorization. For them it can be no other way, since they do not have the tools to understand in a more meaningful way.

We also recommend that instructors return to these principles early and often, reinforcing the underlying concepts rather than expecting students to memorize large databases of reactions.

Organic chemistry is a terminal course in chemistry for many students and is the last time many students will have the opportunity to develop important and worthwhile skills. Students must be asked to construct and explain their answers, so that their thinking can me made clearer, both to themselves and to their instructors. It is well documented, for example, that socially mediated learning provides opportunities for students to explain and construct understanding.⁴ Other approaches may involve explanatory writing^{55,56} and the use of modeling and construction of models of appropriate systems.³⁴ If students are never required to articulate their ideas, it is unlikely that they will have the opportunity to reconstruct them.

Limitations of this study

In this study, we interviewed 17 students and each student provided us with a different combination of models, heuristics, and understanding of the meaning of both words and structures to answer our questions and construct explanations. We do not believe that we have uncovered every potential problem for students or described every student model, but we do think that we have presented a rich picture of the nature of the problem that faces us. We contend that it is not possible, nor is it necessary, to predict all the ways that students use their understandings to construct explanations for these phenomena. What is important is that instructors are aware of the extent of the problem and redesign both curricula and formative assessments to help students explicitly develop and connect these core ideas.

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CHAPTER V: DESIGN AND VALIDATION OF THE INTERMOLECULAR FORCES ASSESSMENT

In the previous chapter, we outlined the various ways that students explain physical and chemical properties of molecular substances. Some students used hydrogen bonding to help explain trends in relative boiling and melting points (although often in a heuristic manner), but few included a discussion of dipole-dipole or LDFs. Students lack of discussion about IMFs led us to further explore their understanding of this topic, particularly because of its essential role in bridging the gap between molecular structure and the resulting physical and chemical properties. If students do not fully understand what IMFs are and where they occur, then it should come as no surprise that these students do not use IMFs to help them reason about properties.¹ This chapter will outline the design, validation, administration, and coding of the Intermolecular Forces Assessment (IMFA), which was created to better understand students' ideas about IMFs through written descriptions and drawn representations.

IMFs interviews: Protocol and findings

Before we could begin designing an assessment to explore students' understanding of IMFs, we first conducted five short interviews to help develop and refine potential questions we could include in our IMFs assessment. While most students discussed IMFs to some degree during our structure-property interviews, few students went into detail about their understanding of the various types of IMFs. Since the main goal of these initial interviews was to investigate how students predict property information using a chemical structure and not necessarily how they viewed IMFs, we decided to conduct an additional five semi-structured interviews to
specifically probe students on their understanding of IMFs. These interviews were conducted with students enrolled in a second-semester organic chemistry course in the summer of 2012 and ranged from 10-20 minutes in length. We used a digital voice recorder as well as a Livescribe pen to record audio and students' drawings.² These students received laboratory participation credit for the interviews and all students signed informed-consent forms.

The interview protocol, shown in Figure 5.1, began by asking students to tell us what they understood about IMFs. We chose to keep this question intentionally broad so that students could reveal their initial ideas about the topic before we inquired about specific IMFs and compounds. Additional follow-up questions were asked about the IMFs they may have mentioned so we could identify how students determined if a given compound was capable of each IMF. We were particularly interested in students' ideas about hydrogen bonding, dipole-dipole interactions, and LDFs as these three IMFs are most commonly covered across general chemistry curricula. After a general discussion of the three main IMFs, we asked students to draw several different types of molecules and discuss any IMFs that may be present. We were specifically interested in how students depicted IMFs. With these interviews we did provide structural guidance to students upon request (with the exception of acetamide, most students did not require assistance) since previous research shows that students have difficulty constructing viable Lewis structures.³

- 1. What is your understanding of the term "intermolecular forces"?
- 2. What features and requirements do you look for to determine if a compound would exhibit a given intermolecular force?
- 3. Can you draw examples of the intermolecular force(s) that you mentioned, using a compound of your choice?
- 4. Can you describe your understanding of the term(s) hydrogen bonding, dipole-dipole, and/or LDFs? (Only if the student did not discuss these specific IMFs on their own earlier in the interview)
- 5. Please draw several water molecules. What IMFs would be present?

a) If a student represented IMFs as occurring within a water molecule, we asked, "Could there be any interaction between two water molecules?"

Question 5 was repeated for ammonia (NH₃), ethane (CH₃CH₃), dimethyl ether (CH₃OCH₃), and acetamide (CH₃CONH₂).

Figure 5.1: Interview protocol for students' understanding of intermolecular forces

Our IMFs interviews, like our structure-property interviews, reinforced the benefit of asking students to provide representations of the topics they discussed. Four of the five students interviewed were able to recall all three types of IMFs and provide a representation for at least two of the three IMFs discussed. Only one of those four students (Rob) required additional prompting about hydrogen bonding to invoke further discussion. We found that the other remaining student, Caitlyn, did not recall any IMFs, even when asked about specific types. Instead she described various reactions when asked about the possibility of interactions between molecules. This was consistent with our previous structure-property interview findings¹ where organic students were more likely to discuss additional (albeit not applicable) ideas from their organic course such as steric hindrance or reaction mechanisms.

The interview protocol—designed from intentionally broad to asking about specific IMFs—appeared to successfully uncover the students' general ideas about hydrogen bonding, dipole-dipole interactions, and LDFs. The students' drawings provided additional context that allowed us to better understand how they viewed IMFs (e.g. as an interaction between

molecules). For instance, Margaery described dipole-dipole as, "something that's going to have a partially negative and a partially positive charge, but...the electron sharing will be a lot more equal." While it was unclear what she meant by electron sharing in her response, her drawing, shown in Figure 5.2, confirmed that she was conflating the idea of dipole-dipole interactions with the bond dipole between two atoms (oxygen and nitrogen). A table containing each student's descriptions and representations of IMFs can be found in Appendix D. Because the drawings proved beneficial during our interviews, we combined questions requiring students to draw with several short answer questions to design a preliminary IMFs assessment.



Figure 5.2: Margaery's depiction of dipole-dipole between oxygen and nitrogen atoms

Designing the initial version of the Intermolecular Forces Assessment (IMFA)

To better explore students' ideas about IMFs we designed an initial version of the IMFA. With this first administration of the IMFA at the beginning of the first-semester of general chemistry (GC1), we wanted to determine what information about IMFs that students brought with them from high school or previous courses about IMFs. Like our interviews, we wanted students to both describe and construct representations of IMFs. In the first version of the IMFA, we provided students with the Lewis structures of four compounds (tetrafluoromethane (CF4), acetic acid (CH₃COOH), propane (CH₃CH₂CH₃), and trimethyl amine ((CH₃)₃N)) since these compounds are capable of a variety of IMFs. For example, while propane only exhibits LDFs, acetic acid is capable of all three IMFs. We then asked students if two molecules of each compound would interact since we did not want to make the assumption that students understood that all molecules we provided interacted in some manner. We then asked them what type of IMFs they would exhibit if they did interact to determine what IMFs they were aware of. Finally, we asked students to provide a molecular-level picture of the interaction they described using three to four molecules. We hoped that, like our interviews, students' drawings would help us better determine their understanding about IMFs. A copy of the pre-instruction assessment with a student's response is provided in Appendix E.

This initial version of the IMFA was given to 66 students enrolled in first-semester general chemistry (GC1). It is important to note that some of these students did receive some instruction regarding LDFs occurring between helium atoms prior to the administration of this pre-instruction assessment. They had not been told, however, that LDFs occur between molecules like the ones included in our assessment. Despite this, several students did reference LDFs in their responses, as discussed below, but this information did not impact any representations of dipole-dipole or hydrogen bonding. The assessment was given on paper in the laboratory setting by teaching assistants and researchers to avoid instructor bias. Students were given participation credit towards their laboratory course for at least attempting to complete the assignment. We were aware that students may not have encountered IMFs before and therefore notified students that it was acceptable to write, "I don't know." All students who participated in the collection of preliminary data signed informed-consent forms.

Of the 66 students who completed the initial IMFA, approximately half (N=35, 53%) did not discuss *any* IMFs in their responses, shown below in Figure 5.3. Instead, common responses included listing covalent and ionic bonds, writing "I don't know", or simply leaving entire sections blank. The remaining students mentioned at least one IMF. The most commonly referenced IMF was hydrogen bonding, however only one student was able to provide an appropriate representation. The remaining students either represented hydrogen bonding as literal

bonds between hydrogen atoms of separate molecules, redrew the molecules provided in an elaborate lattice structure, or offered no representation. LDFs (or Van der Waals forces) were the next most commonly listed IMF. All but one of the students had been exposed to the idea of LDFs during lecture prior to our assessment, so we were not surprised to find discussions of LDFs. Three of the students who mentioned LDFs depicted them as occurring between molecules, however, again most students provided no representation or combined the molecules into a lattice-type structure. Only one student mentioned dipole-dipole, but they did not provide any representation. It is important to note that some students did mention more than one IMF; six listed both hydrogen bonding and LDFs, and one mentioned hydrogen bonding and dipole-dipole.



Figure 5.3: Frequencies of students who did and did not mention IMFs in their pre-instruction intermolecular forces assessment

It is important to reiterate that this was an assessment given pre-instruction, and we did not expect students to show a strong understanding of IMFs. Our main conclusion from this first iteration of the IMFA was that the majority of students either enter general chemistry remembering nothing about IMFs or only remembering specific terms like hydrogen bonding. For many of our students, completing this assessment was an overwhelming process. Asking students to elaborate on topics they do not remember, or were never taught, can be frustrating and cause students to doubt themselves. We found this glaringly apparent in some of the responses we received, like Jason's: "We haven't ever remotely discussed this in my chem class. So it is making me feel stupid." Because of the lack of responses and the unintended stress placed on students who attempted to complete our pre-instruction assessment, we decided that it would be more beneficial to only collect post-instruction data on IMFs in the future.

Redesigning the Intermolecular Forces Assessment (IMFA)

We realized that the questions used in our pre-instruction assessment did not require students to discuss their understanding of IMFs. In fact, we had only asked them to provide a list of IMFs that would be present for a series of compounds. We felt it was important to ask students to describe their understanding of IMFs, both generally and in terms of specific IMFs. Simply being able to identify or list the IMFs that would be present for a given compound might not necessarily reflect a solid understanding of IMFs. As a result, when revising the IMFA we continued to further draw upon our previous IMFs interviews, specifically probing students understanding of each IMF and allowing them to describe compounds capable of interacting through those IMFs.

With these questions as a guide, we redesigned the IMFA to first ask students about their general understanding of IMFs and to then list all of the IMFs that they knew of. Like our earlier IMFs interviews, we then asked students to provide example compounds that would exhibit those IMFs. In case students did not discuss the three IMFs we were specifically interested in, in their previous responses, we asked about their understanding of hydrogen bonding, dipole-dipole, and LDFs.

Like both the interviews and the initial IMFA, we wanted students to construct representations of IMFs for a given compound. In our first IMFA attempt, we provided students with four different structures and asked them to construct representations of interactions. This proved to be rather time consuming and repetitive for students, thus we decided for our redesign to focus on a single compound and ask students to draw out and clearly label each IMF. Water was initially discussed as a possible compound to use but ultimately we decided against it; most students are overly familiar with water (it is often the quintessential example used to explain hydrogen bonding). Instead, we chose to use ethanol because it is capable of all three IMFs and is less complex than structures we had used previously like acetic acid or trimethyl amine. We included the chemical formula (CH₃CH₂OH) to provide some guidance for students drawing the ethanol structure. We did not want students to mistakenly draw dimethyl ether (a valid structure for C_2H_6O) or other non-ethanol structures. We did not provide students with the Lewis structure for ethanol in the IMFA because we wanted students to have the freedom to use a representation of their choice (e.g. particulate, bond-line, etc.). An example of Item 7, asking students to construct representations of hydrogen bonding, is provided below in Figure 5.4.



Figure 5.4: An example of item 7 on the IMFA

We learned from our pre-instruction IMFA administration that collecting student responses through a paper medium has its disadvantages, particularly when storing and reviewing student work. Therefore, we chose to complete the redesign of the IMFA and administer it using the online platform *beSocratic*.^{4,5} *beSocratic* is an interactive program that allows for free-form student input through writing, drawing, and constructing graphs. It can also be used for more traditional methods of input, such as multiple-choice or fill in the blank questions. By using *beSocratic*, we could easily collect students' text and drawing responses in a single, online assessment as well as code and export responses using the system's analysis tools. Additionally, *beSocratic* gave us the ability to prevent students from returning to previous questions in the IMFA and editing their responses as they progressed through the assessment and were given additional pieces of information.

Pilot testing the redesigned IMFA

Once we created our redesigned IMFA on *beSocratic*, we gave the assessment to three second-semester general chemistry (GC2) students in an interview setting to finalize instruction wording and make sure that students interpreted each question as intended. We made minor wording changes to address feedback given by the students. We then pilot tested the redesigned IMFA with 68 GC2 students in the middle of the Spring 2012 semester. All of these students had been instructed, and tested, on IMFs so the information discussed in the IMFA should have been familiar to them. The redesigned IMFA pilot test was administered in the laboratory setting on *beSocratic* using tablet PC's. This ensured that students could easily draw structures using the provided stylus. By collecting responses outside of the lecture setting, we hoped to remove (or at least lessen) any instructor influences. The IMFA pilot test was administered by teaching assistants (TA's) and research assistants (RA's); no instructors were involved in the pilot test data collection.

Finalizing the IMFA design

We did not encounter any major difficulties during the pilot-testing phase and thus began collecting from a larger population of students at the end of the Spring 2012 semester (N=181). The IMFA was administered to students enrolled in either general chemistry or organic chemistry at Clemson University. As in our pilot test, TA's and RA's administered the IMFA to students in the laboratory setting to remove instructor bias. Student responses were collected through *beSocratic* using tablet PC's and iPads.

We made two additions to the IMFA after our Spring 2012 data collection. Some students expressed frustration in having to describe specific IMFs, like hydrogen bonding, if they had

already provided an explanation in a previous question. In response, we added an option to items

4-6 for students to write "see previous" if they had already discussed a specific IMF.

Additionally, due to the ambiguity of some students' drawings and feedback we received from

students in our Spring 2012 data collection, we chose to add a text box to items 7-9 to allow

students to describe anything they were unable to represent in their drawings. Most students have

not used this feature, but we have kept it in the IMFA for clarification during the coding process.

The final version of the IMFA is included below in Figure 5.5. A timeline of the IMFA design

and data collections is provided below in Figure 5.6, including collections from organic

chemistry 1 (OC1) and 2 (OC2) students.

- 1. What is your current understanding of the term "intermolecular forces"?
- 2. List all types of intermolecular forces that you know of below and please define each.
- 3. Please give example(s) of a compound that would exhibit the intermolecular force(s) that you listed previously. Be sure to list the intermolecular force(s) that the compound is representing.
- 4 6. What is your current understanding of the terms hydrogen bonding, dipole-dipole interactions, and London dispersion forces?
- 7 9. Please draw and label a representation below that clearly indicates where the hydrogen bonding is present for three molecules of CH₃CH₂OH. In the box, please describe, in words, anything you were unable to adequately represent in your drawing. If you do not think this interaction is present, please write, "not present".
- Items 8 and 9 are similarly phrased and ask for representations of dipole-dipole and London dispersion forces respectively.

Figure 5.5: Intermolecular Forces Assessment^{6,7}



Figure 5.6: IMFA data collections

IMFA coding and validation

Student drawings (Items 7-9)

At the end of our first large data collection in the Spring of 2012, we began to devise a coding scheme for the IMFA. The IMFA contains nine assessment items; in order to narrow down the amount and type of responses we would need to code, we chose to initially focus on students' drawing responses to items 7-9. These three items essentially form the heart of the IMFA, and research has shown that students' representations can provide an additional lens through which we can view their understanding of IMFs.^{8,9} Three researchers, myself, a postdoctoral researcher, and a faculty member, used *beSocratic*'s "code replay" function to create codes from students' drawings. This function allows researchers to replay a student's submission and apply a code at a desired time point. For our purposes, we were mainly interested in the final representation a student provided, rather than the process they used to achieve that representation. That is, while we did replay a handful of student responses, codes for students' drawings of IMFs were applied at the end of the replay rather than at a specific time point during the replay. Additionally, by using *beSocratic* to both collect and analyze student data, we were able to gather all responses from one administration in a single location. *beSocratic* automatically applies an anonymous identifier to each student to prevent bias on behalf of the researcher and allows for blind coding. It is only after coding is finished and exported that researchers can identify which students are enrolled in a particular course.

We began our analysis of student drawings with hydrogen bonding (item 7) in *beSocratic*. From our interviews and IMFA pre-instruction data collection, we had some understanding of what students' representations might look like in terms of IMF location (i.e. that students might represent IMFs as within or between molecules). Because of this, parts of our

coding scheme were more deductive than inductive. That is, we used our prior work to inform the creation of our codes related to IMF location.¹⁰ We did use an open-coding, inductive approach to create additional fine-grained codes unrelated to IMF location.¹¹ Our initial, fine-grained codes are shown below in Figure 5.7(a) and (b). It quickly became apparent, based on the codes created, that there were two initial key categories. Because of our previous research, approximately half of the codes created related specifically to the location of IMFs (as intended). The remaining codes developed from an open-coding approach mostly related to the structure used by students to represent ethanol.



Figure 5.7: (a) and (b) Initial codes created for students' representations of hydrogen bonding (IMFA item 7)

Figure 5.8(a), shown below, outlines our initial reorganization of these codes into larger categories such as hydrogen bonding occurring "within" molecules or "between" molecules. With this iteration of coding, we still believed it was important to determine where an IMF was specifically located, and thus we maintained the fine-grained location codes within the larger location categories. At this coding stage, we also reorganized our structural codes to change the

focus from structural features to the type of representation used, shown in Figure 5.8(b). We noticed students used a variety of representations and felt that this should be represented in our coding scheme. This involved the creation additional codes to encompass representations beyond Lewis structures such as particulate and condensed structures. We also created an additional code category called "number of molecules" during this coding iteration, shown in Figure 5.8(c). Our instructions in the IMFA explicitly asked students to include three molecules of ethanol but we noticed students who drew only one (or none) for their representations of hydrogen bonding. By introducing this category, we were curious to see how many students drew one molecule or less (which would make it rather difficult to represent IMFs as *between* molecules).



Figure 5.8: (a) early reorganization of location codes into categories; (b) addition and organization of structure codes; (c) addition of the number of molecules codes

After applying these coding categories to students' responses during the Spring 2012 administration of the IMFA, we decided to refine and consolidate our coding to focus solely on the location of the IMF in students' representations. We chose to discontinue the "number of molecules" category when coding future IMFA data collections because of the strong overlap between this category and the location category. For example, students who drew only one molecule most often also received a "within" molecule code, so the "number of molecules" category did not enhance the coding of students' representations. We also decided to discontinue the coding for the type of representation used by students in their depictions of IMFs. While we did find some variation in how students represented ethanol, the type of representation used by students rarely affected how they depicted the location of the IMF. There was no correct representation that we expected students to use, and while most students favored Lewis structures, previous research within our group had already explored students' difficulties in constructing these structures.³

We chose to focus primarily on the location code because we felt that the location category truly addressed the defining feature of IMFs: that they occur *between* small molecules. The distinction between bonds and IMFs is an important one and thus the location theme became the predominant coding scheme for all subsequent IMFA administrations. The final "location" category used consisted of the following codes: "within" molecules, "between" molecules, "ambiguous" location, "not present", and "student DK" (student does not know). We decided to subsume the fine-grained location codes (shown in Figure 5.8(a)) into the larger location codes, thus only coding for the five main location codes. Examples of student drawings of hydrogen bonding that received these location codes can be found in Figure 5.9(a) – (e). It should be noted that drawings of hydrogen bonding (or any other IMF) that receive a "between" molecules code may not necessarily be a correct representation. For instance, a student may indicate that hydrogen bonding occurs between hydrogens on two ethanol molecules.



Figure 5.9: Student representations of hydrogen bonding that received (a) between code, (b) within code, (c) ambiguous code, (d) not present code, and (e) student DK code

Similar representation and location codes were applied to students' drawings of dipoledipole interactions and LDFs. Specifically, the same location codes were used for students' dipole-dipole representations, but an additional code was added for LDFs. When coding students' drawings of LDFs, we found several instances of students stating that this particular IMF was "always present" or "everywhere". Indeed, all molecules are capable of exhibiting LDFs so the discussion of LDFs as occurring everywhere is somewhat understandable. Students who provided this explanation instead of a representation of LDFs received an "always present" code for location of the IMF. Examples of students' drawings of dipole-dipole and LDFs that received each location code can be found in Appendix F.

In order to determine inter-rater reliability of the location coding scheme, another graduate student and I coded a random subset of 30 student drawings for hydrogen bonding,

dipole-dipole, and LDFs. We exhibited 100% agreement in our coding of students' hydrogen bonding and dipole-dipole drawings, resulting in a Cohen's kappa value of 1. Additionally, we achieved a Cohen's kappa value of 0.96 for our coding of students' drawings of LDFs.

Student text (Items 2, 4-6)

After completing the location coding scheme for students' drawings of IMFs, we turned to their written responses in search of a discussion of location. Specifically, we wanted to explore how their discussion of location in their text responses compared to the locations provided in their representations. This meant that, unlike our coding of students' drawings, our approach for coding students' text responses was significantly more constrained; we purposefully mirrored our location drawing scheme when developing codes for student writing. As a result, our main writing location codes, shown in Figure 5.10, were "within" molecules, "between" molecules, and "ambiguous" (listed in Figure 5.10 as other). In order to receive a "within" or "between" code, students needed to *explicitly* state the location of the IMF. By using similar coding schemes, we hoped to highlight similarities and differences between the two types of response modalities.

We used *beSocratic's* "code text responses" feature to highlight sections of relevant text and apply codes. In order to streamline coding of students' written responses from items 2 and 4-6, we exported their text and recombined them based on the IMF discussed. So, for example, a student's discussion of hydrogen bonding from item 2 would be combined with their discussion of hydrogen bonding from item 4 to create a complete description within a single response. We then imported these consolidated responses back into *beSocratic* for text coding. Figure 5.10

shows an example of a consolidated student response as well as the coding scheme used for their writing.



Figure 5.10: Example of a consolidated students' response for hydrogen bonding and location coding scheme

To determine inter-rater reliability of the location coding scheme for students' text responses, another graduate student and I coded a random subset of 40 student written responses for hydrogen bonding and LDFs. This resulted in an initial Cohen's kappa of 0.87 and 0.58. We identified discrepancies in how each coder was determining which LDFs text responses would result in a "within" molecules code as opposed to "ambiguous". For example, one coder identified the response "temporary dipoles in molecules create a weak force" as LDFs occurring within the molecule while another coded it as "ambiguous". Upon further discussion, it was decided that, despite mentioning dipoles within the molecule, it was unclear from the students' responses if they believed LDFs actually occurred within the molecule or were simply influenced by dipoles within the molecule. Unless a student explicitly stated that an IMF occurred within a

molecule, they received an "ambiguous" location code. Researchers achieved a Cohen's kappa value of 1 for all three codes after further negotiation. A faculty member and I coded a random subset of students' dipole-dipole text responses resulting in a Cohen's kappa value of 0.95.

IMFA data collections

To date, the IMFA has been administered at two universities, Clemson University and Michigan State University, and a residential college within Michigan State University. We have collected responses from students enrolled in GC1, GC2, OC1, and OC2. We have also collected IMFA data longitudinally, following a small group of student from general chemistry through organic chemistry. All of our administrations of the IMFA are shown in Figure 5.6. Results from bolded collections in Figure 5.6 are discussed in greater detail in the next two chapters. The first chapter will compare traditional students' responses about IMFs based on question modality, while the next chapter will show the effect of a reformed general chemistry curriculum on students' understanding of IMFs in comparison to those enrolled in a traditional course. It will also explore students' responses from different universities and examine the consistency of students' IMFA responses over time. REFERENCES

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CHAPTER VI: STUDENT UNDERSTANDING OF INTERMOLECULAR FORCES: A MULTIMODAL STUDY

Preface

This chapter discusses findings from our research on how students write about and represent IMFs. This research has been previously published in the Journal of Chemical Education as an ACS Editor's Choice article and is thus available for copying and redistribution or any adaptations for non-commercial purposes. Reprinted with permission from:

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Words are useful for representing certain kinds of material – perhaps representations that are more formal and require more effort to translate – whereas pictures are more useful for presenting other kinds of material – perhaps more intuitive, more natural representations. In short, one picture is not necessarily equivalent to 1,000 words (or any number of words). - Richard Mayer¹

Introduction

The importance of intermolecular forces

The study reported here is part of a series of studies on students' understanding of structure and property relationships.^{2–6} Our goals for this research are to: (i) investigate the difficulties that students have and (ii) develop assessment strategies for the steps involved in learning to use structures as models to predict and explain properties. Our ultimate goal is to use the data from these investigations to develop evidence-based approaches to teaching and learning that will improve understanding of this important construct. In this study, we focus on student understanding of intermolecular forces (IMFs), specifically hydrogen bonding, dipole-dipole interactions, and London dispersion forces (LDFs). As we have previously noted,³ the pathway that connects a molecular structure to the properties of a substance requires a long chain of inferences. Ideally, a student should be able to construct and then use a structure (by understanding that the shape and electron distribution in the molecule determine molecular polarity) to make deductions about interactions between molecules (intermolecular forces) that govern both physical and chemical properties. Each of these tasks is difficult in itself³ and connecting them to make predictions about properties is highly demanding for students. In essence, we are asking students to move from using Lewis structures as representations to using them as models with which they can predict and explain properties.⁷ If this shift in perspective is not made explicit to students, then even the simple task of constructing the representation may become difficult for many students because they may not see the purpose of drawing structures. Students' knowledge of structure-property relationships is not conditionalized and is therefore often inert; that is, their knowledge is not useful for this purpose. For example, we have shown that even organic students struggle to construct Lewis structures¹ and have proposed that, while a rules-based approach to structure drawing provides a deceptively easy way to teach this skill, if students do not understand *why* they are learning to draw structures then the tenets for meaningful learning^{8,9} are not met and students do not connect and reinforce skills that do not seem relevant to them. This is supported by our findings that, even after organic chemistry, many students do not understand how to use Lewis structures to predict anything other than surface-level features of a molecule.^{2,3} Many students have not progressed from the idea of a structure as a representation to the idea of a structure as a model.

In another study⁴, we interviewed students about how they used structural representations to predict properties. In this environment, where prompting and further elicitation of student ideas was possible, it became clear that, for many students, structure and properties were not explicitly connected. Typically, students tended to rely on heuristics and surface-level features of molecules to make predictions rather than using the sequence of inferences that they had been taught. In this study⁴, students usually did not use IMFs as a construct to help them reason about properties such as relative boiling points, even when specifically asked probing questions designed to elicit such ideas. Although some students used terms such as hydrogen bonding or London dispersion forces, few students used them in anything other than a rote fashion. Only two students invoked London dispersion forces to explain the difference in boiling point of methanol and ethanol, while most instead relied on rules such as "the more bonds the higher the boiling point", which was sometimes coupled with the idea that covalent bonds break during phase changes.⁵ This finding supports the work of Talanquer and coworkers who have reported that heuristic reasoning is prevalent in a range of tasks such as identifying acids and bases¹⁰ and predicting relative melting and boiling points and solubility.¹¹ Since many students did not seem

to understand the need to incorporate IMFs into their reasoning about bulk properties of molecular species, we decided to investigate what students do understand about IMFs.

Prior work on student understanding of IMFs

The study described here is the first of a series of papers¹² designed to probe students' understanding of intermolecular forces and how students write about and construct representations of IMFs; that is, the interactions between separate molecules that govern the properties of those molecules such as boiling point and acid-base reactivity. Prior research involving IMFs has focused specifically on hydrogen bonding^{13–15}—perhaps because of its importance in the properties of water and in biological systems—or more broadly on the general topic of IMFs.^{16,17} Most of these studies have found that some students are (perhaps understandably) confused about the nature of the hydrogen bond. We should not be surprised when students have difficulties with the difference between covalent bonds and intermolecular forces, especially when they are exacerbated by the fact that an intermolecular force is named "bond". For example, Henderleiter and coworkers interviewed students about their understanding of hydrogen bonds and found that, of the 22 organic students, four of them indicated that the hydrogen bond was the covalent bond between an O and H in the same molecule.¹³ Similarly, Peterson and coworkers, using a two-tier multiple choice diagnostic test, reported that 23% of grade 12 high school students indicated that intermolecular forces were the forces within a molecule.¹⁶ Using this same diagnostic test, other researchers found that 35% of students in Singapore also displayed this idea.¹⁷ While there are other well-documented problems with student understanding of hydrogen bonds (for example that any molecule containing hydrogen and oxygen can hydrogen bond¹⁴), it is the notion that an intermolecular force such as hydrogen bonding is actually a covalent bond that is most problematic.

If students believe that IMFs are interactions within molecules, this idea must affect their models of phase change. For example, if a student learns that water has a relatively high boiling point because the strong hydrogen bonds must be overcome, then we should not be too surprised when students' phase change models revolve around breaking actual covalent bonds.^{5,13,14,18–20} Barker and Millar found that while the students they studied from age 16 through 18 improved in their understanding of hydrogen bonding over time, none of the students in the study invoked any other IMFs to explain trends in boiling point.¹⁸ As discussed earlier, our own work has supported this finding and extends it to students at the college level in general and organic chemistry.⁵ Schmidt and coworkers reported that upper secondary school students in Germany had great difficulty predicting boiling points of organic compounds and very few (15%) used appropriate reasoning when asked to explain their answer to a multiple-choice question.¹⁴

This paper describes an investigation into the external representations that students use to communicate about IMFs. Rather than hoping to prompt discussion of IMFs in a context with a phenomenon such as predicting relative boiling points (as we had done previously and which we now know is unlikely to happen⁵), we wanted to ask students specifically about their understanding of IMFs. As noted, earlier studies with IMFs have most often used forced-choice instruments.^{14–17} Although it is impossible to "know" exactly what a student understands, it is important to use the best evidence available to draw conclusions.²¹ For us, this means having students construct their own responses rather than restricting them to choosing an answer from a list. While multiple-choice items and diagnostic two-tier instruments are fast and reliable, it has been shown that students can answer these questions without recourse to appropriate scientific thinking.²² For example, previous research has shown that students were able to rank the boiling

points of a range of compounds without thinking about intermolecular forces^{4,18} and instead used heuristics that may have led them to the correct answer but were scientifically flawed.

Theoretical perspective

The importance of multimodal learning, that is providing both visual (pictures) and verbal (words) support for student learning, has long been emphasized. It has been proposed that instructional materials providing both words and pictorial representations are more effective because student understanding can be enhanced by the addition of non-verbal knowledge representations.²³ However, there is less research on how students use multimodal (pictorial and verbal) representations to explain and represent their understanding. It has been proposed that drawing can provide a "window into student thinking" and there are a number of studies^{24–29} that have investigated the effectiveness of drawing in support of learning in science. Drawing should be particularly helpful in identifying student ideas about spatial information; for example, understanding how they view the relative positions of molecules and the forces that act between them.

Similarly, having students write about their understanding can also provide useful insights into student thinking. Certainly both modalities require students to construct answers and thus make their ideas explicit. There are several studies that compare two groups of student responses: those who draw and those who write. For example, Gobert and Clement compared responses for student who drew diagrams or produced text summaries about plate tectonics.³⁰ Similarly, Akayagun and Jones looked at the ways that students wrote about or constructed representations of equilibrium systems.³¹ Both studies found that the representations students constructed tended to emphasize different features than the written explanations. However, in

neither study were students asked to both write and draw so it was not possible to compare a particular student's textual explanations and drawings.

Our goals with this study were to investigate how both writing and drawing about IMFs can provide us with insight into how students understand this concept. Therefore, students were asked to both construct a representation of an IMF (i.e. draw three structures of ethanol to show how they interact) and discuss their understanding of that particular IMF in words. That is, we asked students to use more than one modality to answer questions about IMFs in hopes that it would provide us with a more nuanced picture of their understanding than either writing or drawing alone.

The study was designed to address three research questions:

RQ1: How do students represent IMFs in free-form drawings?

RQ2: How do students discuss and describe IMFs in open-ended written responses?

RQ3: How do students' written explanations compare to their drawn representations?

Methods

Student population

The participants in this study consisted of a subsample of students from a larger population of 1600 students enrolled in general chemistry at a mid-sized public southeastern research university (Cohort 1, Fall 2011–Spring 2012, N = 94). An additional cohort from the following year was included in this study for replication purposes (Cohort 2, Fall 2012 – Spring 2013, N = 160). The freshman population at this university is approximately 48% female and 52% male with the majority of students, 84%, identifying as white. The average ACT score for incoming freshman ranges from 26 to 31 and the mean SAT score is 1246. While the general chemistry course at this university was traditional in content (i.e., taught using a commercially available text), the course had been revised to include a more conceptual approach and some sections of the courses

employed reformed pedagogies such as the use of clickers and in-class group quizzes. Students also completed online homework assignments using a commercially available homework system (Mastering Chemistry³²). The common examinations for these courses were exclusively multiple-choice and, at the end of a full academic year, the American Chemical Society (ACS) nationally normed general chemistry examination³³ was administered as the final exam. Students in this course typically score around the 75th percentile on the ACS general chemistry exam. All the students included in this study consented to participate in this research by signing informed consent forms. Demographic information for each cohort is provided in Appendix I.

Development of the Intermolecular Forces Assessment (IMFA)

The Intermolecular Forces Assessment (IMFA)^{*} was designed to elicit students' understanding of IMFs by asking them a range of questions that probe the way students think about IMFs. It was developed based on responses from interviews with general chemistry and organic chemistry students where students discussed how they used structural representations to help them understand phase changes.⁵ The representations that students constructed along with their verbal descriptions provided us with insight into how the students were thinking about these processes. Interim versions of the IMFA were piloted in student interviews and revised for clarity where necessary. The final version (Figure 6.1) was administered to 68 students in a pilot study and was then used in the studies reported here.

^{*} The development and design of the IMFA is further addressed in Chapter 5.

Intermolecular Forces Assessment

- 1. What is your current understanding of the term "intermolecular forces"?
- 2. List all types of intermolecular forces that you know of below and please define each.
- 3. Please give example(s) of a compound that would exhibit the intermolecular force(s) that you listed previously. Be sure to list the intermolecular force(s) that the compound is representing.
- 4–6. What is your current understanding of the terms hydrogen bonding, dipole-dipole interactions, and London dispersion forces?
- 7–9. Please draw and label a representation below that clearly indicates where the hydrogen bonding is present for **three** molecules of CH₃CH₂OH. In the box, please describe, in words, anything you were unable to adequately represent in your drawing. If you do not think this interaction is present, please write "not present".

Items 8 and 9 are similarly phrased and ask for representations of dipole–dipole and London dispersion forces, respectively. An example showing the question layout is included in Supporting Information.

Figure 6.1: Items included on the Intermolecular Forces Assessment

The IMFA is designed to explore how students think about and represent IMFs. Items 1–3 ask students for general examples and explanations of IMFs without any specific prompts. In this way, we are able to capture students' spontaneous responses without prompting them about a particular IMF. For example, students are asked to explain what they understand by the general term intermolecular forces, which IMFs they know about, and to provide an example of a substance that would exhibit those IMFs. In items 4–9, students are asked specifically about hydrogen bonding, dipole-dipole and London dispersion forces, both by explaining what they understand by these terms (items 4–6) as well as constructing drawings or representations (items 7–9) that would show the presence of specific IMFs (if present).

Note that students were explicitly asked to draw three molecules and the term **three** was bolded, since in early iterations of the IMFA many students drew only one molecule. Ethanol was selected as the target for these items because it is a relatively simple molecule that is capable of exhibiting hydrogen bonding, dipole-dipole, and London dispersion forces (LDFs). Students were asked to draw structures of ethanol, but were given structural cues (CH₃CH₂OH) so that most students in this study were able to construct a reasonable (recognizable) representation.

The IMFA was administered to both cohorts of students at the end of their second-semester of general chemistry (GC2) to ensure that all students had been exposed to, and tested on, the relevant material. The IMFA was administered outside of lecture in the laboratory setting (which students take concurrently with lecture). Students received participation points for at least attempting to complete the IMFA. None of the instructors for the course were involved in data collection or analysis process. Research and teaching assistants collected all student responses on iPads and tablet PC's using the online software platform *beSocratic*, which allows collection of both free-form student drawings and text inputs.^{34,35} That is, we asked students to both draw representations of IMFs and explain the IMFs in words. Using this system, we prevented students from returning to any prior items once they moved forward so that students were not able to alter their answers as they progressed through the assessment. In this study, we focus on the student responses to items 2 and 4–9. Drawings (items 7–9) from both Cohorts 1 and 2 were analyzed, and written responses (items 2, 4, 5, and 6) were analyzed for Cohort 1.

Data analysis: Drawings (Items 6–9)

The students' responses were analyzed using post-analysis tools in *beSocratic*.^{34,35} The program records each student's drawing input step-by-step, allowing the researcher to replay a student's response at a later time. The coding feature in *beSocratic* was used to code and store

important actions or features of the drawing. An open-coding, constant comparison approach was used to develop an analysis scheme for students' IMF drawings.^{36,37} Three researchers (a graduate student, a post-doctoral researcher, and a faculty member) analyzed and discussed the set of codes created from the open-coding process and agreed that there were only a few, distinct ways that students represented IMFs. The major code categories that emerged for drawings of each type of IMF were: within, between, ambiguous, and not present. If a student clearly indicated that the IMF occurred within a molecule (i.e. circling or pointing to a particular covalent bond) the drawing was coded as "within", while a "between" molecules code meant that a student made an indication that the IMF was located between two molecules, typically by marking the space between ethanol molecules (see Table 6.1 for examples using drawings of hydrogen bonding).

IMF Type	Code for IMFA Response Drawings Characterizing IMF Locations			
	Within the Molecule	Between Molecules	Ambiguous	
Hydrogen Bonding	H H H Hydrogen H - C - C - O - H Hydrogen H - H H - H M - H	M H Mond - O - C - C - H I - C - C - O - H H - C - C - O - H H - C - C - C - H H - C - C - C - H H - C - C - C - H H - H - H H - H - H H - H - H H - O - C - C - H H - H H - O - C - C - H H - H H - H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - O - C - C - H H - H H - H H - O - C - C - H H - H H - H H - H H - H H - O - C - C - H H - H - H H	H H H H H H H H H H H H H H H H H H H	
Dipole– Dipole Interaction	-0-н -5 5 раз топ ста хони	H H H H H H H H H H H H H C-C-C-H H H H C-C-C-H Interactions	H H H-C-C-O-H H H H H	
LDFs	H H C - C - C - C - C - C - C - C - C -	London disperson LH3CH20H ES CH3CH20H CH3CH30H ES CH3CH30H ES CH3CH30H ES CH3CH30H ES	CH3CH2OH CH3CH2OH CH3CH2OH CH3CH2OH	

Table 6.1: Coding examples for student drawings demonstrating understanding of selected types of intermolecular forces

If the location of an IMF was not clearly specified (i.e. within or between), the response was coded as "ambiguous". An explicit indication that the IMF was not present received a "not present" code. In rare cases, a student might indicate an IMF as both a bond within a molecule as well as occurring between molecules. These students received a "within and between" code. A code used only for the question about LDFs, "states always present" was added because some students, rather than providing a representation, described (in words) that LDFs are something that all substances are capable of or is always present for compounds. Some students indicated in words that they were unsure how to answer the question or represent the structures. A "Student DK" (does not know) code was added. Examples of the codes "within", "between", and "ambiguous" for dipole-dipole and LDFs are provided in Table 6.1.

It should be noted that the codes "within" or "between" do not indicate whether a student's representation of the IMF was completely correct. For example, a student might indicate that the hydrogen bonded to carbon in the ethanol molecule would hydrogen bond with the oxygen of another ethanol molecule. In this analysis, the student would receive a "between" code for their depiction, even though their representation of hydrogen bonding is incorrect. We did analyze the "correctness" of the students' representations of hydrogen bonding. However, analyzing drawings for correctness of dipole–dipole and LDFs was more challenging because students may represent charge distribution or fluctuating dipoles in many different ways, or not include indications of the role of charges at all. Even variations in structural representations, such as Lewis structures, condensed structures, or particulate representations can blur the lines between what can effectively be considered "correct" versus "incorrect". Therefore, we do not report "correct" for these two IMFs.

To determine the inter-rater reliability of the analyses, one of the authors and another graduate student coded a random sample of 30 student drawings for each IMF giving a Cohen's Kappa of 1.0 for hydrogen bonding and dipole-dipole drawings, and a Cohen's Kappa of 0.96 for LDFs.

Data analysis: Text responses (Items 2, 4–6)

Student text responses collected from items 2, 4, 5, and 6 were analyzed using the coding scheme we developed from the students' drawings as a guide. The text responses for item 2 (where students were asked in general to identify types of IMFs) were combined with the specific items 4–6, since many students wrote more detailed responses in item 2 and simply referred to their prior responses in items 4–6. For this study, each text response was coded specifically for a discussion of the *location* of the IMFs. That is, the text was analyzed to see

whether the student discussed IMFs as occurring "within" the molecule or "between" molecules and was coded as "ambiguous" if the location was not specified. Using a similar approach for both the students' drawings and explanations allowed us to investigate in what ways students' text responses corresponded to their drawn representations. Examples of text responses and the corresponding codes are shown in Table 6.2.

IMF	Pseudonym	Quote	Text code
Hydrogen Bonding	Tracey	"When the hydrogen atom from a molecule that has a large difference in electronegativity (i.e., hydrogen and oxygen) is attracted to a negative portion of another molecule."	Between
	Lindsay	"The strongest types of intermolecular forces and a hydrogen atom must be bonded to another hydrogen, nitrogen, oxygen or floride [<i>sic</i>]."	Ambiguous
Dipole– Dipole	Adelaide	"Stronger than London dispersion forces and occurs between two polar molecules"	Between
	Laura	"Intermolecular force in which dipoles within the molecule are attracted to each other and hold the molecule togetherstronger than LDFs"	Within
	Marta	"Exhibited when the compound it [<i>sic</i>] polar, Its the second strongest"	Ambiguous
LDFs	Ann	"Forces between all molecules that get stronger with increasing molecule size."	Between
	Rebel	"Are present in all molecules. Small attractive forces."	Ambiguous
	Casey	"The weakest that are found in every molecular bond"	Within

Table 6.2: Examples of text codes applied to Cohort 1 students' responses for each IMF

To determine the inter-rater reliability of the analyses, one of the authors and a graduate student coded a random sample of 40 student text responses for both hydrogen bonding and LDFs, initially resulting in a Cohen's Kappa of 0.87 and 0.58 respectively. Researchers further discussed the coding scheme for LDFs to clarify what categorized a response as "within" a molecule or "ambiguous". For example, the response "temporary dipoles in molecules create a weak force" was originally coded as "within" by one coder and "ambiguous" by the other. After discussion, it was determined that, while the student did mention dipoles within the molecule, it was not apparent where the student considered the weak force to be located. If a response did not explicitly state that *LDFs* were located within a molecule, then it could not be coded as "within". Both sets of codes resulted in a Cohen's Kappa of 1.0 after negotiation between researchers to clarify any discrepancies. Two of the authors coded a random sample of 40 dipole–dipole responses giving a Cohen's kappa of 0.95.

Results and discussion

RQ1: How do students represent IMFs in free-form drawings?

The analysis of Cohort 1 students' drawings of hydrogen bonding, dipole–dipole, and LDFs (items 7–9) are shown in Figure 6.2. Of the 94 GC2 students who completed the IMFA, only 15% (N = 14) of students correctly indicated that hydrogen bonding occurs **between** separate molecules. Of these students, only nine were completely correct in showing the hydrogen bonding interaction between an H (bonded to an O) in one molecule and an O in another molecule.

Of the remaining students, 72% (N = 68) clearly represented hydrogen bonding as an O—H bond within a single molecule of ethanol. In fact, 54% (N = 51) of students drew only one molecule or none at all (even though they were explicitly asked to draw three molecules). All but three of the drawings coded as within clearly depicted the IMF as the covalent O—H bond within a molecule of ethanol. While the idea that the term "hydrogen bonding" refers to the covalent oxygen–hydrogen bond within the molecule has been previously documented, the
extent of this error has not. As discussed earlier, previous studies have shown a much lower



prevalence of this idea ranging from 23-35% of students.^{13,16,17}

Figure 6.2: Code frequencies for students' representations of IMFs from Cohort 1 and Cohort 2

While it is quite understandable that students might be confused about the term "hydrogen bonding", since the term "bond" is misleading, we found that student confusion extended to representations of both dipole–dipole and LDFs as well. Again only a small number of students drew dipole–dipole (11%, N = 10) and LDFs (12%, N = 11) as interactions between molecules. As we saw with hydrogen bonding, the majority of students (61%, N = 57) in Cohort 1 drew dipole–dipole interactions as occurring within the ethanol molecule and as did 55% (N = 52) for LDFs. Students' depictions of dipole–dipole and LDFs were somewhat more varied than those for hydrogen bonding. For example, in Table 6.1 (within, dipole–dipole) all of the C—H bonds are depicted as dipole–dipole interactions. Representations of LDFs include circling individual atoms (such as hydrogen in Table 6.1 (within, LDFs)), lone pairs of electrons on oxygen atoms, or bonds. In fact, of the students in Cohort 1 who drew LDFs occurring within the molecule,

seven students circled every bond in the ethanol molecule, which may be related to the idea that "every substance has LDFs".

The IMFA was also administered to a second cohort of general chemistry students (Cohort 2) in the following year, and the results are also shown in Figure 6.2. While there was a slight increase in the number of Cohort 2 students who drew representations of hydrogen bonding and LDFs occurring between molecules, again the majority of these students' representations for hydrogen bonding (56%, N = 90), for dipole–dipole (58%, N = 93), and for LDFs (56%, N = 89) clearly indicated that the IMFs were located within a single molecule. We attribute the slight improvement to the fact that the instructors in the courses were now aware of our results for Cohort 1 and had emphasized IMFs more than usual in the following year.

RQ2: How do students discuss and describe IMFs in open-ended written responses?

Written responses about hydrogen bonding, dipole–dipole, and LDFs (items 2, 4–6) were analyzed for the students in Cohort 1 (N = 94), using a coding scheme similar to that for their drawings. Unlike the drawings where the location of IMFs, as either within a molecule or between molecules, was usually quite obvious, students' text responses were typically less explicit. Of the 94 students in Cohort 1, only 4% (N = 4) of students explicitly stated that IMFs occur between molecules for all three types of IMFs. Similarly only a few students stated explicitly that IMFs occur within a single molecule. Specifically, 5% (N = 5) of students stated that dipole–dipole occurred within a single molecule and only one student claimed that LDFs did the same. None of the students in Cohort 1 explicitly stated that hydrogen bonding occurs within a molecule. Indeed most students failed to make any reference to the location of IMFs at all, meaning that most responses received the ambiguous text code, as shown in Figure 6.3. It should be noted that an ambiguous code did not mean that a student's response was incorrect, but rather that it was missing a discussion of the location of the IMF.



Figure 6.3: Code frequencies for students' representations of IMFs from Cohort 1

Lindsay's ambiguous response for hydrogen bonding, shown in Table 6.2, is typical in that the elements involved and the strength of the IMF are discussed. Similarly, many students (for example, Rebel) provided ambiguous responses for LDFs. Not represented in the Figure 6.3 are the 26% (N = 24) of students who explicitly stated in their written responses that LDFs are present for all molecules or always present. We suspect that this response may stem from students hearing their instructors talk about LDFs in a similar fashion. While it is true that all molecules are capable of interacting via LDFs, it is easy to imagine that students may understand this as a property of the molecule rather than of the interactions between molecules.

Interestingly, the written responses about dipole–dipole interactions did not follow the same pattern as those for hydrogen bonding and LDFs. A much larger group of Cohort 1 students (49%, N = 46) stated explicitly that dipole–dipole interactions occurred between molecules, shown in Figure 6.3. As discussed below, this is in contrast to the students' representations of dipole–dipole interactions where a majority of students drew structures showing dipole–dipole

interactions *within* a particular molecule (Figure 6.2). While we do not know the reason why more students wrote about dipole–dipole interactions between molecules, like the responses for H-bonding and LDFs, the responses were somewhat superficial. It may be that the students had learned a definition of dipole–dipole that specifically included the idea that the interaction was between molecules.

One factor that made student written responses difficult to interpret was that students often appeared to use words without understanding their meaning. In addition to the term "intermolecular", students often used atom to mean molecule (or vice versa) and bond to mean IMF (or vice versa). For example, Rueben, as shown in Table 6.3, refers to a molecule of fluorine when discussing hydrogen bonding but he probably meant to describe an atom. This interchanging of atom and molecule has been in reported previously in work by Cokelez and Dumon.³⁸ The confusion between atom and molecule is fairly obvious here, but this mistake may not always be so clear. A student who confuses these terms might discuss an interaction between atoms but mean an interaction between molecules-an important distinction. Additionally, some students used the terms bond and interaction interchangeably. While a bond is a type of interaction, we usually do not refer to IMFs as bonds (except, of course, for hydrogen bonds!). Thomas, for example, discusses a bond between molecules but it is unclear whether he understands the difference between the terms bond and interaction and whether he is using the appropriate one in this scenario. Since student use of terminology can be imprecise, it can make it difficult to know what students mean from their writing alone, which often resulted in the students' text responses being considered ambiguous. Additional quotes from students where terminology becomes problematic are shown in Table 6.3.

Terminology issue	IMF	Pseudonym	Quote	Text code	Drawing code
Atom vs. Molecule	Hydrogen Bonding	Georgia	"hydrogen bonding- between a hydrogen atom on one molecule and either an oxygen, nitrogen, or fluorine of another atom"	Ambiguous	Between
		Rueben	"hydrogen bonds: a molecule of fluorine [<i>sic</i>], oxygen, or nitrogen bonded with a hydrogen"	Ambiguous	Within
		Regina	"Hydrogen bonds- an intermolecular force between a hydrogen atom and either an O or F molecule"	Ambiguous	Within
Bond vs. Interaction	Dipole– Dipole	Thomas	Dipole-dipole is "a pretty weak bond between polar molecules."	Between	Within
		Ray	"Dipole-Dipole- bond between two molecules that is nonpolar"	Between	Ambiguous
	LDFs	Betty	LDFs are "A very weak bond that binds any two molecules, or parts of any two molecules, together."	Between	Ambiguous

Table 6.3: Examples of terminology issues in student responses

RQ3: How do students' written explanations compare to their drawn representations?

Drawing and writing provide different approaches to eliciting student understanding and our use of similar codes for both modalities allowed us to compare the text and drawn responses. Most students constructed a drawing of an IMF showing its location explicitly within a single molecule, coupled with an ambiguous text description (for hydrogen bonding: 70%, N = 66; and LDFs: 48%, *N* = 45). Only 3% of students in Cohort 1 gave what would be considered an "ideal" answer for the location of hydrogen bonding by explicitly stating that hydrogen bonding occurred between molecules *and* drawing an interaction occurring between molecules. Comparisons of the major categories for drawing and written explanations are shown in Figure 6.4. We include here the "other" category, which also incorporates such answers as "not present" and "I don't know". All combinations of text and drawing responses from students are provided in Appendix J.



Figure 6.4: Comparison of Cohort 1 students' code frequencies for text and drawings of IMFs

As discussed earlier most students were not specific about the location of IMFs in their written explanations; in fact, 93% (N = 87) of students' written responses for hydrogen bonding received an ambiguous code (Figure 6.3). It is only when we look at the drawings of hydrogen bonding that we can see what students are trying to explain. For example, Tobias and Maeby have similar explanations of hydrogen bonding, as shown in Table 6.4. It would be difficult to

distinguish between their responses (knowing as we do that the term intermolecular is often misunderstood by students), without looking at their drawings, which show that Tobias understands hydrogen bonding as interactions between molecules, while Maeby does not.

Pseudonym	Drawing	Quote
Tobias	H - C - C - O - H H - C - C - O	Hydrogen bonding is "an intermolecular force between hydrogen and N O F. It is the strongest intermolecular force."
Maeby	H H H H H H H O H Within Molecules	Hydrogen bonding is "between hydrogen and oxygen, nitrogen, and fluorine"

Table 6.4: Drawing and text comparisons for Tobias and Maeby

Similarly for LDFs, the drawings provided more information than the writing. Consider, for example, Oscar and Rita in Table 6.5. Oscar described LDFs as "the simplest and weakest of the IMF" and Rita indicated that LDFs were "present in all molecules, but the one force in polar molecules. The weakest of the three". Again, upon viewing their drawings, it becomes clear that Oscar has an understanding of LDFs as interactions between separate molecules, while Rita does not.

Pseudonym	Drawing	Quote
Oscar	H-C-C-O-H H-O-C-C-H H-O-C-C-H H-H H-H H-O-C-C-O-H H-H H-H H-H H-C-C-O-H H-H H-C-C-O-H H-H H-C-C-O-H	LDFs are "the simplest and weakest of the IMF"
Rita	HELDEH HAILbonds have it blr molecules Within Molecules	LDFs are "present in all molecules, but the one force in polar molecules. The weakest of the three"

Table 6.5: Drawing and text comparisons for Oscar and Rita

Just as with hydrogen bonding and LDFs, few students (9%, N = 8) correctly described dipole–dipole as an interaction between molecules *and* provided an appropriate representation (Figure 6.4). Unlike hydrogen bonding and LDFs, however, 49% (N = 46) of students in Cohort 1 provided text responses for dipole–dipole that described the interaction as taking place *between* molecules (Figure 6.3). Despite this, 28% (N = 26) of Cohort 1 drew an explicit representation of dipole–dipole interactions as occurring *within* a molecule of ethanol while at the same time describing the interaction as occurring *between* molecules in their written response (Figure 6.4). For instance, Gene described dipole–dipole as an "intermolecular force formed between two dipole molecules that comes from different electronegativities". Even so, his drawing, seen in Table 6.6, clearly shows dipole–dipole interactions as C—H bonds in one molecule of ethanol. Perhaps more important to note is that, while many students' written responses by themselves might be interpreted as correct, it is only when we consult the students' representations that we can see whether they understand the "intermolecular" part of intermolecular forces. By drawing, students are able to show us where they believe these interactions occur²⁴ and, as a result, show aspects of their understanding that are not captured in their written descriptions.

Pseudonym	Drawing	Quote
Trisha	Dirole - dirole interactions Between Molecules	Dipole–dipole is "between molecules that have positive and negatively charged ends. The different ends are attracted to each other"
Gene	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \end{array}\\ \end{array}\\ \end{array}\\ \end{array}\\ \end{array} \\ \begin{array}{c} \end{array}\\ \end{array} \\ \end{array} \\ \begin{array}{c} \end{array}\\ \end{array} \\ \end{array} \\ \begin{array}{c} \end{array}\\ \end{array} \\ \begin{array}{c} \end{array}$ \left(\begin{array}{c} \end{array}\\ \end{array} \\ \begin{array}{c} \end{array}\\ \end{array} \\ \begin{array}{c} \end{array}\\ \end{array} \\ \begin{array}{c} \end{array} \left(\begin{array}{c} \end{array}\\ \end{array} \\ \end{array} \\ \begin{array}{c} \end{array} \left(\begin{array}{c} \end{array}\\ \end{array} \left(\begin{array}{c} \end{array}\\ \end{array} \left(\begin{array}{c} \end{array}) \\ \end{array} \left(\begin{array}{c} \end{array} \left(\begin{array}{c} \end{array} \left(\begin{array}{c} \end{array} \left(\end{array}) \\ \end{array} \left(\begin{array}{c} \end{array} \left(\end{array}) \\ \end{array} \left(\begin{array}{c} \end{array} \left(\end{array}) \\ \end{array} \left(\end{array} \left(\end{array} \left) \\ \end{array} \end{array} \end{array} $ \begin{array}$ $ \begin{array}$ } $ \begin{array}$ } $ \end{array}$	Dipole-dipole is an "intermolecular force formed between two dipole molecules that comes from different electronegativities"

Table 6.6: Drawing and text comparisons for Trisha and Gene

Summary

The three main findings of this study follow:

First, drawings of IMFs collected in this study indicate that a majority of students draw representations showing that IMFs are located within a single molecule rather than between separate molecules (Figure 6.2). Although this finding is similar to previous studies in which students confuse IMFs and covalent bonds within a molecule^{13,16,17}, the results presented here contrast with prior studies where a much smaller percentage of the students (certainly less than a majority) exhibited this misunderstanding. There are several possible explanations for this finding; perhaps the most obvious is that these students have not been taught appropriately. However, these students are representative of a cohort who averaged around the 75th percentile

on the ACS general chemistry examination. We also have some evidence¹² that while the student response is highly dependent on the learning environment, the finding that many students depict intermolecular forces as interactions within a molecule is not unusual for a traditionally sequenced general chemistry course.

Most of the previous reports on student understanding of IMFs rely on forced-choice assessments, in which some of the responses may not even address the particular problem of inter- versus intra-molecular forces. For example, in Schmidt and colleagues' study of student understanding of IMFs,¹⁴ several items were of the type "In which of the following compound(s) is hydrogen bonding likely to occur between the molecules?" which would, of course, preclude the idea that hydrogen bonding occurs within a molecule. Villafañe and colleagues developed a multiple-choice instrument using clusters of questions designed to probe topics important to the development of students' understanding of biochemistry.¹⁵ Their assessment included three items designed to address how students understand hydrogen bonding. It is significant that this cluster of items had the lowest Cronbach's alpha coefficient, 0.306, indicating a weak correlation between students' responses to the three items. Only 12% of the students in their study gave completely correct responses to all three items in the hydrogen bonding cluster.²¹

Second, in contrast to their drawings, students' writing about IMFs was more ambiguous (Figure 6.3). While most students' responses clearly indicated an attempt to discuss the IMF provided in the prompt, many were paraphrases of textbook definitions: for example, listing the elements involved in hydrogen bonding, or indicating that all molecules are capable of London dispersion forces. Very few students specifically indicated that intermolecular forces occur between molecules or discussed the origin of intermolecular forces as electrostatic interactions. While this may have been a consequence of the lack of specificity of the prompt, in this study it

was not possible to determine from student writing whether students have an appropriate conception of IMFs.

Third, comparison of student writing and drawing indicates that drawings are much easier to categorize. For the most part, students' written descriptions were ambiguous, while their drawings were not (Figure 6.4). In fact, we provided some examples within this paper that show student discussions may have been considered "correct" but were paired with a representation that would be incorrect: for instance, Maeby's response in Table 6.4 or Gene's in Table 6.6. We believe that student-constructed representations can provide more insight into student understanding, particularly with respect to spatial information such as the location of IMFs.

Conclusions

It is clear from inspection of student drawings that many students have problematic ideas about intermolecular forces. For each IMF, more than half of the students in both cohorts drew representations that explicitly showed an interaction within a molecule, yet student written descriptions were often much more ambiguous or, in the case of dipole–dipole, contradictory. The fact that the majority of students drew pictures indicating each IMF as interactions within a molecule leads us to believe that, like many other concepts, student understanding of IMFs is highly problematic, fractured, and unstable.^{5,39–41} Depending on the nature of the prompt, we may elicit differing and often contradictory ideas. Because of this, we must be particularly careful not to draw conclusions from single assessment items. Clearly it is important to provide students with opportunities to construct responses in multiple formats and to help them reconcile differences between their responses.

Implications for teaching and future work

The fact that a majority of students can emerge from a general chemistry course without a consistent understanding that intermolecular forces operate between molecules is highly problematic. Intermolecular forces mediate much of chemistry, from the temperature at which phase changes occur, to solubility and reactivity. The well documented "misconception" that covalent bonds break when a phase change occurs^{5,13,14,18–20} becomes more understandable in light of this finding. As we have previously noted, determining which IMFs are present within the bulk substance are part of a long sequence of ideas and skills that students must construct for themselves before they can understand structure-property relationships. Clearly one approach to helping students might be to emphasize the teaching of IMFs more in general chemistry courses. Inspection of a number of popular texts, including the one used by students in this study (General Chemistry: Atoms First by McMurray and Fay⁴²) shows that the topic of IMFs is clearly explicated with well-designed and clear representations. However, knowledge is not transferred intact (either from a text or in a lecture), but is instead constructed by the student.^{43,44} Clear exposition and repetition of important ideas are not sufficient to produce a robust and useful understanding. In fact, in many general chemistry courses the topic of IMFs is often separated both from the prior knowledge that is needed to understand it (i.e., molecular structure, shape, and polarity) and from the material for which IMFs are needed to understand a concept (e.g., solubility and phase changes). That is, the teaching of IMFs does not meet the tenets for meaningful learning in that prior knowledge, instruction, and the purpose of that knowledge must be explicitly connected.^{8,43} Knowledge must be contextualized before it becomes useful.⁴⁵ While this study looked at IMFs using small molecules as our substrate, we must also bear in mind that

non-covalent interactions mediate much of biological chemistry from protein folding to enzyme substrate interactions.

It is our contention that, to develop a robust understanding, the curriculum must be restructured to emphasize the connections between important ideas and that students must be given opportunities to reflect on and make their thinking visible.⁴⁶ That is, students must have the opportunity to construct and revise representations, models, and explanations that allow them to predict and explain phenomena. Otherwise, it becomes too easy to assume that students have learned important concepts because they can choose the correct answer on an examination. Indeed one might wonder why the extent of this problem has gone unrecognized for so long. It may well be that our increasing reliance on homework using online course management systems and multiple-choice tests has contributed to the problem. If students are not ever asked to write and draw, to reflect, to explain, and to revise their ideas, but instead are only assessed by which item they choose on a test or randomly generated homework, it is unlikely that they will develop a robust and coherent understanding of core concepts. This is not to say that multiple-choice items are never useful (indeed they are almost unavoidable in large enrollment courses), but that students must also be given many opportunities to construct answers for themselves as they learn.

One further note, some authors have recommended that intermolecular forces such as hydrogen bonding or London dispersion forces be considered as bonds⁴⁷ and there is a compelling argument that bonds and intermolecular forces be considered part of a continuum of interactions between atoms. However, it is crucial that students also understand the differences. That is, when an IMF is overcome, the result is typically not a new chemical substance but rather a phase change (or in the case of large molecules a change in conformation or shape). When

bonds are broken, new chemical substances are produced with different properties and arrangements of atoms. These differences, while quite apparent to the expert, are clearly not so obvious to students. It is our contention that students who do not have a firm grasp on the forces that act both within and between molecules will be unable to make sense of phase changes, solution formations, and chemical reactions. While experts may point out that the word "intermolecular" actually defines where the forces act, it has been well documented, both in this study and in other reports, that students have difficulty using terminology appropriately.^{38,48}

Our future work on helping students understand and use IMFs focuses on two areas. The first is investigating how changes in learning environment affect the ways that students represent and understand intermolecular forces. In a follow-up paper in this series,¹² we present a comparison between matched cohorts of students from traditional and transformed courses. We also are collecting data from a wider range of institutions and instructional settings. The second area of research is to develop more nuanced approaches to eliciting the ways in which students think about IMFs and their role in bulk properties of matter, including designing scaffolded prompts to elicit student beliefs about how IMFs are formed and how they are linked to properties. We believe that a major goal of chemistry education is to help students develop causal, mechanistic explanations of phenomena, and understanding IMFs is crucial to this goal.

Limitations of the study

The IMFA was designed to require students to first write about their understanding of IMFs and then provide constructed representations of those IMFs. We did not ask students to justify or explain their drawings and what they intended to show. Because of this, we had to infer students' intentions from their drawings alone.

The study reported here was performed at one institution and it might be argued that the institutional setting was such that the results are not applicable to other institutions. However, in future papers we will be reporting similar studies from multiple institutions and with multiple types of courses, and we have reason to believe that the data presented here are not a "worst case scenario".

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CHAPTER VII: ARE NON-COVALENT INTERACTIONS AN ACHILLES HEEL IN CHEMISTRY? A COMPARISON OF INSTRUCTIONAL APPROACHES

Introduction

The question of how to improve student learning in chemistry has long been debated. Since the earliest 1920's, authors have proposed improved ways to teach particular topics or to restructure courses.^{1–5} However, these earlier efforts were hampered by several factors, including a lack of appropriate assessments and a dearth of research on teaching and learning guided by theories of learning. Therefore, although it was not for lack of effort, it was difficult to provide strong evidence about effective strategies, interventions, or curricular innovations designed to improve specific aspects of student learning. Over the past twenty years or so much more evidence has been gathered about how people learn⁶ and, more specifically, what problems students encounter when they learn chemistry.^{7,8} Despite this, there is still sparse evidence about strategies that have actually improved student understanding and use of specific concepts. Most of the current approaches to improve teaching and learning focus on making the classroom more student-centered,^{9,10} and there is now a good deal of evidence that these techniques can improve student success and persistence in a particular course.¹¹ The measures of such success, however, are typically grades in the course, performance on nationally-normed examinations, or multiplechoice concept inventories.^{11,12} Much of the chemistry education research literature describes student difficulties and misconceptions^{7,13} and, while many authors also provide a section on implications for teaching and learning, there is scant evidence that these findings have made their way into mainstream courses in a way that shows they have improved student understanding. At the same time, there is a great deal of evidence that even students who perform well in our

courses and above average on nationally-normed tests may develop profound misunderstandings of core concepts in chemistry during instruction and are often unable to explain these concepts or transfer their ideas to new situations.^{7,14,15}

In our current work^{14–18}, we are using both research on student difficulties and theories of learning to design, implement and assess evidence-based approaches to improving student learning. In this chapter, we describe the effects of a curriculum transformation designed to help students develop a robust understanding of structure-property relationships and present evidence of students' improved understanding of an important linking concept for structure-property relationships: intermolecular forces.

Intermolecular forces

We have previously shown that many students, who perform well on traditional assessments, have profound misunderstandings about intermolecular forces (IMFs).^{14,19} In particular, we found that a majority of students in our studies constructed representations of IMFs showing them as interactions within (rather than between) molecules. We believe that one reason this problem has been under-reported for so long is because of the nature of the assessments used to probe student understanding of IMFs. For example, one study on student ideas about hydrogen bonding uses items such as "In which of the following compound(s) is hydrogen bonding likely to occur between the molecules?"²⁰ That is, there is an assumption that understanding which substances can exhibit hydrogen bonding is evidence that the student understands what hydrogen bonding is and where it occurs. This is almost certainly an invalid assumption for many students. Most prior studies on how students understand IMFs use either multiple-choice instruments or short answer assessment items. For example, studies employing a

two-tier diagnostic test found that around 30% of students tend to have a problematic understanding of IMFs as forces within a molecule, rather than between.^{21,22} Others have focused on hydrogen bonding and have also reported problematic ideas, particularly around the notion that the O—H covalent bond is the hydrogen bond.^{20,23} While confusions about the nature of hydrogen bonding are quite understandable (the name itself is misleading), there are fewer studies that include other types of intermolecular forces, such as London dispersion forces or dipole-dipole interactions.^{24,25}

We developed the Intermolecular Forces Assessment (IMFA), discussed in Chapter 5, to investigate student understanding of IMFs by requiring students to construct representations and to explain in words what they understand about each IMF.¹⁹ The IMFA was previously administered to students using our online platform *beSocratic*, which allows us to collect, record and analyze both student writing and drawings.^{26,27} We found that only *one* student out of 94 in our previous study was consistently able to represent all three intermolecular forces (hydrogen bonding, dipole-dipole and LDFs) as interactions between separate molecules.¹⁹ In general, about 55% of each student cohort tended to represent IMFs as interactions within a single molecule by, for example, drawing a molecule and circling one or more bonds. We also found that much of what students wrote about IMFs was ambiguous; indeed without the student-generated drawings as further evidence it would not have been possible to determine whether students understood that intermolecular forces are forces between molecules rather than within.

This result was surprising and perturbing. The students involved were successful students in a well-designed traditional general chemistry course where students average around the 75th percentile on the ACS general chemistry examination.²⁸ If a majority of students do not have a working understanding of the difference between IMFs and chemical bonds, it should not be

surprising when we find that students believe that bonds break during phase changes^{14,20,23,29,30} or that they have trouble developing reaction mechanisms.^{31–34}

Developing improved understanding in a reformed curriculum

Cooper and Klymkowsky have previously reported on the development of a new general chemistry curriculum, Chemistry, Life, the Universe and Everything (CLUE).³⁵ This curriculum is based on a carefully scaffolded progression of three core ideas: structure, properties and energy. Each core idea is developed over the yearlong sequence and is connected simultaneously and explicitly to the other core ideas. Scientific practices³⁶ such as constructing explanations, arguments and models are emphasized. At the same time, we developed an online system (*beSocratic*) that allows us to ask students to explain phenomena and construct diagrams and models by drawing and writing in response to prompts.^{26,27}

Our current work focuses on assessing how the CLUE curriculum affects student performance and understanding. We have previously reported¹⁶ on a comparison of students' ability to draw and use Lewis structures for matched cohorts of CLUE and traditional students. We found that CLUE students were significantly better at drawing Lewis structures and were also more likely to self-report that these structures could be used to predict both chemical and physical properties¹⁶ using the Implicit Information from Lewis Structure Instrument (IILSI), a self-report instrument.¹⁷ That is, CLUE students were more likely to recognize that structural representations could be used to predict and explain properties than traditional students.

In this chapter, we continue this study with an investigation of how CLUE and traditional students compare in their representations of intermolecular forces. In our studies using the IILSI, we found that by the end of general chemistry both CLUE and traditional students were equally

likely to indicate that they could predict the types of intermolecular forces a substance would exhibit.^{16,37} However, the IILSI is a self-report instrument and, although recognizing that IMFs can be predicted from structures is an important first step, it does not mean that students actually understand what IMFs are. We, therefore, turned to the newer assessment instrument, the IMFA¹⁹, in which students are asked to draw three molecules of ethanol and show the location of each intermolecular force (hydrogen bonding, dipole-dipole and LDFs). They are also asked to explain what they understand about each IMF and to explain anything they cannot portray in their drawings. The details and design of the instrument are reported in Chapter 5.

Research Questions

- How do CLUE students' representations of IMFs compare to students enrolled in a traditional general chemistry course?
- 2. How do students at different institutions compare in their representations of IMFs?
- 3. How do CLUE and traditional students' representations of IMFs change over the course of the subsequent organic chemistry course?

Methods

Student populations and study design

The Intermolecular Forces Assessment (IMFA) was administered at two universities. Clemson University is a medium-sized, southeastern public research university with an average fall enrollment of 1600 students in first-semester general chemistry (GC1). Subsequently, approximately 600 students enroll each fall in organic chemistry. In the fall of 2012, the composition the 3400-student freshman class of Clemson was approximately 52% male and 48% female with the freshman population being predominately white (84%). The mean SAT score for incoming freshman was 1246 with an average ACT range of 26-31. Michigan State University (MSU) is a large, midwestern public research university with a fall enrollment of approximately 2500 students in first-semester general chemistry. The freshman class at MSU in 2013, consisting of over 7000 students, was approximately 48% male and 52% female. As with Clemson, the freshman population at MSU was predominately white, at 76%, with an average ACT range of 23-28.

While both universities are research intensive with comparable student populations and demographics, there are some differences in course requirements and learning environments between Clemson and MSU. First, about 65% of students at Clemson take both semesters of general chemistry (GC) sequentially from fall to spring semester, unlike MSU where this percentage drops to around 30%. Second, the typical size of the lecture course ranges from 100-170 at Clemson and from 350-430 for MSU. The general chemistry course at MSU also has a recitation component where students are encouraged to work additional problem sets and seek assistance from graduate teaching assistants. Lastly, at Clemson the general chemistry lecture and laboratory sections are listed as a single course, while at MSU, the general chemistry lecture and laboratory are separate courses and, in fact, most students do not take the GC lab course concurrently with lecture.

The IMFA was administered to two cohorts of students (Cohort 1 and 2) enrolled in introductory chemistry courses at Clemson and an additional cohort of students (Cohort 3) enrolled at MSU. These cohorts consist of students who have completed the first semester of general chemistry and are enrolled in the second-semester of general chemistry (GC2). Additionally, students from Cohort 1 were followed through two years, from first-semester

general chemistry through the second semester of organic chemistry (OC2). Student populations

for each cohort can be seen in Table 7.1.

Table 7.1: Student populations for each cohort at Clemson University and Michigan State University

Clen	MSU	
Cohort 1	Cohort 2	Cohort 3
(Fall 2011 – Spring 2013)	(Fall 2012 – Spring 2013)	(Fall 2013 – Spring 2014)
Traditional GC: N=94		
CLUE GC: N=87		
Longitudinal Study (through	Traditional GC: N=160	Traditional GC: N=239
<i>OC</i> 2):	CLUE GC: N=117	CLUE GC: N=187
Traditional N=25		
CLUE N=30		

Study 1: A comparison of CLUE and traditional students at Clemson University

Cohorts 1 and 2 from Clemson consisted of two groups of students: those enrolled in both the first (GC1) and second semester (GC2) of the CLUE general chemistry course or the traditional general chemistry course. The traditional general chemistry course at Clemson uses a widely available general chemistry textbook.³⁸ Learning objectives are provided for traditional students and course examinations are designed to address multiple representations and concepts as well as testing facility with calculations and other skill-based questions. Many of the traditional lecture sections are designed to be interactive with students answering clicker questions, taking group quizzes, and participating in in-class activities. Students complete the American Chemical Society's (ACS) standardized general chemistry exam at the end of GC2 and typically score around the 75th percentile.²⁸

We used a quasi-experimental control-treatment design.³⁹ CLUE students in both Cohort 1 and Cohort 2 were directed towards the CLUE lecture sections of the course because of their intended majors in biological sciences or pre-professional health studies, but a number of other majors, including engineering, were also enrolled. The traditional comparison groups for both Cohorts 1 and 2 were selected from the larger general chemistry population of students enrolled in the traditional course. For Cohort 1, traditional students were selected based on their similarity to the CLUE student population in major, sex, SAT composite score, Metacognitive Activities Inventory (MCAI) scores⁴⁰, Student Understanding of Models in Science (SUMS) scores⁴¹ and Implicit Information from Lewis Structures Instrument (IILSI) scores¹⁷. Traditional students in Cohort 2 were selected based on their similarity to the CLUE population in major, sex, SAT composite score, MCAI scores, and responses to the IILSI (further details are listed in Appendix K). CLUE students in Cohorts 1 and 2 had different lecture instructors for the course, both of whom were familiar with the design and implementation of the CLUE curriculum.

IMFA responses were collected from Cohort 1 and Cohort 2 at the end of GC2 in order to ensure that all CLUE and traditional GC students had been exposed to, and been assessed on, the topic of intermolecular forces. Student responses were collected outside of the lecture setting in the laboratory course, which runs concurrently with the lecture. Since there is an inherent conflict of interest when assessing the effects of a reform designed by the research team, it was important to separate the data collection from the lecture as much as possible. Neither of the CLUE lecture instructors was involved with data collection. Students received credit (laboratory participation points) for at least attempting to complete the assessment. The IMFA was administered by research assistants not involved with the lecture course using *beSocratic*, a webbased system that allows for free-form student input such as written text responses, drawings, and constructed graphs.^{26,27} The data were collected on tablet PC's and on iPad's since both allow for drawing with a stylus and typing written responses.

Study 2: A comparison of CLUE and traditional students from different universities

Cohort 3 consists of CLUE and traditional GC students enrolled at MSU. It is important to note that, for Cohort 3, we do not have a matched control group to make statistical comparisons between instructional approaches. In this chapter, we are presenting the analysis of CLUE student responses to provide preliminary evidence of how the curriculum transfers from one institution to another. We also include the traditional student responses in a comparison to those from Clemson to address additional difficulties experienced by students. As with Cohorts 1 and 2, student responses for Cohort 3 were collected at the end of GC2 after all students had been taught, and tested, on intermolecular forces. Since students are not required to take the laboratory course concurrently with lecture at MSU, student responses were instead collected by research and teaching assistants during recitations using the *beSocratic* program on iPad's or tablet PC's. Recitations are directly tied to the lecture course and the teaching assistants leading recitation work closely with the lecturer for the course. Therefore, the data collection at MSU is more closely tied to the lecture section and the instructor of the course. The CLUE instructor for Cohort 3 at MSU is the same instructor who taught CLUE Cohort 1 at Clemson.

Study 3: A longitudinal study of students' representations of IMFs

While the majority of our data from Clemson was collected from students enrolled in general chemistry, we also followed a subset of general chemistry students in Cohort 1 who continued on through both sequential semesters of organic chemistry (OC1 and OC2) to investigate how student representations of IMFs changed in subsequent courses. In this study, the IMFA was administered again at the end of OC2. Since most majors at Clemson do not require students to take more than one year of chemistry, many students do not go on to enroll in organic

chemistry, therefore our CLUE and traditional groups by the end of OC2 were significantly smaller (N = 30 and N = 25, respectively). For this study, we compared the results for only this smaller subset of students who had completed *all* administrations of the IMFA.

Data coding and analysis

The studies discussed here focus on student drawings; as we have previously reported most students' written responses to the prompts in the IMFA are typically ambiguous in regards to the location of IMFs.¹⁹ Therefore, we chose to code the drawings only, which provided us with a much less ambiguous representation of students understanding about IMFs. As in our prior study, the three major codes for each IMF are *between* (molecules), *within* (molecules) and *ambiguous* as shown in Table 7.2.

ME type	Code for IMFA response drawings characterizing IMF locations			
nvn [,] type	Within the molecule	Between molecules	Ambiguous	
Hydrogen Bonding	H H H H H H H H H H H H H H H H H H H	$\begin{array}{c} H & H \\ H - C - C - O - H \\ H - L \\ H \\$	L-L-AH U-L-L U-L-L IC Th A QVUN Draw Erse N XRest	
Dipole– Dipole Interactions	$\begin{array}{c} H \\ H $	$\begin{array}{c} \begin{array}{c} & & & \\ & & & \\ H - \left(- \frac{1}{2} \right)^{2} \cdot \frac{1}{2} \cdot \frac{1}{2} \\ & & \\ H - \frac{1}{2} \right)^{2} \cdot \frac{1}{2} \cdot \frac{1}{2} \\ & & \\ H - \frac{1}{2} \right)^{2} \cdot \frac{1}{2} \cdot \frac{1}{2} \\ & & \\ H - \frac{1}{2} \right)^{2} \cdot \frac{1}{2} \cdot \frac{1}{2} \\ & & \\ H - \frac{1}{2} \right)^{2} \cdot \frac{1}{2} \\ & & \\ H - \frac{1}$	H3 H2 H H3 H2 H H3 H2 H H2 H2 H Draw Erase · XReset	
LDFs	Draw Frace × XRest	8 5 5 8 5 8 + Draw Erase • XReset	H H H $- 2 - 2 - 0 - H$ H H H H H H H - 2 - 2 - 0 - H H - 2 - 2 - 0 - H H H H H - 2 - 2 - 0 - H H H H H - 2 - 2 - 0 - H	

 Table 7.2: Coding examples for student drawings of selected types of intermolecular forces

While the codes shown above were the most prevalent, a "within and between" code was applied to representations that clearly indicated an IMF as occurring both within a molecule as well as between molecules. Students were also asked to write "not present" if they believed ethanol was not capable of exhibiting a particular IMF, resulting in a "not present" code. Some students indicated that they were unsure how to answer, so a "Student DK" (does not know) code was created. Finally, an additional code, "always present", was used exclusively for LDFs because some students, rather than providing a representation indicating the location, wrote that LDFs are always present, or occur everywhere. For the purpose of clarity, we will present the "within molecules" and "between molecules" data below, since these codes account for the majority of responses in our study. The full data sets are available in Appendix L.

Results and discussion

Study 1: Results and discussion – Clemson University, Cohorts 1 and 2, GC2

As shown below in Figure 7.1 and Table 7.3, there is a significant difference between the representations of IMFs locations from CLUE students and those in the traditional general chemistry class for both Cohorts 1 and 2. In general, the majority of CLUE students draw *all* types of IMFs as interactions between molecules, while the majority of traditional students draw them as within individual molecules. Specifically, 83% (N=72) of CLUE students in Cohort 1 and 84% (N=98) from Cohort 2 drew hydrogen bonds *between* molecules. Of the 72 Cohort 1 CLUE students who drew hydrogen bonding between molecules of ethanol, 96% (N=69) correctly indicated the location between the oxygen of one molecule and the hydrogen covalently bonded to oxygen on another molecule. That is, not only did the majority of CLUE students

correctly depict hydrogen bonding as occurring between molecules, but almost all of them provided what would be considered a correct representation of hydrogen bonding between appropriate elements on each molecule. Only 10% of CLUE students in both Cohort 1 (N=9) and Cohort 2 (N=12) provided an incorrect representation of hydrogen bonding as a covalent bond within a molecule of ethanol. These data are shown in Figure 7.1.



Figure 7.1: Comparison of code frequencies for students' representations of hydrogen bonding, dipole-dipole, and LDFs from Cohort 1 and Cohort 2

As we have previously reported¹⁹, however, 72% (N=68) of traditional GC2 students in Cohort 1 and 56% (N=90) of traditional students in Cohort 2 indicated that hydrogen bonding occurred *within the molecule* as seen in Figure 7.1. This pattern, where CLUE students represent IMFs between molecules and traditional students indicate they are bonds within a molecule, was not limited to hydrogen bonding. The majority of CLUE students' representations of both dipoledipole (63%, N=55 for Cohort 1 and 72%, N=84 for Cohort 2) and LDFs (62%, N=54 for Cohort 1 and 68%, N=80 for Cohort 2) also showed IMFs as interactions between molecules. Similarly, the majority of traditional students' representations depicted dipole-dipole (61%, N=57 for Cohort 1 and 58%, N=93 for Cohort 2) and LDFs (55%, N=52 for Cohort 1 and 56%, N=89 for Cohort 2) as occurring within the ethanol molecule. For each of the three IMFs, at least 55% of the traditional students' representations from Cohort 1 and 2 depicted all IMFs as a bond within a single ethanol molecule. At most only 31% (N=50, Cohort 2) of traditional students ever provided a depiction of hydrogen bonding as located *between* molecules, and even fewer represented dipole-dipole and LDFs as occurring between molecules, as shown below. While Figure 7.1 shows the most common codes, within and between, applied to student drawings, *all* code frequencies for all Cohort 1 and 2 responses are included in Appendix L.

As shown in Table 7.3, significant differences were identified between the CLUE and traditional groups' drawing code frequencies for both within and between molecules. These differences were found for all three IMFs in both Cohorts 1 and 2. Code frequencies were analyzed using chi-square statistics and effect sizes (ϕ) are included. Effect size values greater than 0.3 are considered a medium effect size and those greater than 0.5 are considered large.⁴² Major codes that resulted in statistically significant differences between the two groups are included in Table 7.3. Additional codes, including ambiguous, not present, and always present, are included in Appendix L.

Table 7.3: Statistical results for comparing code frequencies for CLUE and Traditional students' IMF drawings at the end of GC2 in Cohort 1 and Cohort 2. p-values from chi-square analysis are reported along with calculated effect sizes (ϕ , phi coefficient)

Cohort	IMF	Code	Traditional	CLUE	p-value	ø
			percentage	percentage		Ŷ
Cohort 1	Hydrogen	Within	72.3	10.3	< .001	0.62
	bonding	Between	14.9	82.8	< .001	0.67
	Dipole-dipole	Within	60.6	13.8	< .001	0.47
		Between	10.6	63.2	< .001	0.54
	LDFs	Within	55.3	14.9	< .001	0.41
		Between	11.7	62.1	< .001	0.51
Cohort 2	Hydrogen	Within	56.2	10.2	< .001	0.46
	bonding	Between	31.3	83.8	< .001	0.51
	Dipole-dipole	Within	58.1	16.2	< .001	0.41
		Between	15.6	71.8	< .001	0.56
	LDFs	Within	55.6	12.8	<.001	0.43
		Between	20.0	68.4	<.001	0.48

The findings from Cohort 1 and 2 for both CLUE and traditional students are very similar despite the fact that different instructors taught CLUE each year and that the traditional students were chosen from sections taught by at least five different instructors. We believe that the persistent differences we see here are a result of the curriculum, not a function of student ability or the instructor.

Consistency of responses for Cohort 1

While Figure 7.1 depicts the percentage of students who received within or between codes for each IMF, it does not show whether these students are *consistent* in the way they represent IMFs. That is, a single student could have drawn hydrogen bonding as occurring within a molecule, but provided ambiguous drawings for dipole-dipole and LDFs. We used Sankey diagrams^{43,44}, which are a type of flow diagram, to visualize whether students' representations were consistent. Figure 7.2 shows two Sankey diagrams, the first for traditional students in Cohort 1 and the second for CLUE students in Cohort 1, to show how the representations

provided by each student change (or do not change) between all three IMFs. The width of the pathways represents the number of students who took that path. Although the diagram can only show how students change between two consecutive IMFs, it does indicate that there is a lack of consistency for many students. For example, 10 traditional students who received a within code for hydrogen bonding then stated that dipole-dipole was not present for ethanol. However, the diagram does not show what codes those 10 students received next for LDFs. But we can see, for *all* students who stated, "not present" for dipole-dipole, what codes they received for LDFs in their subsequent drawing.



Figure 7.2: Flow chart representing the consistency of code frequencies applied to student drawings in Cohort 1, both traditional and CLUE, across all three IMFs

Ideally we would like to see that students have a consistent understanding of all IMFs as interactions between molecules. While at least 60% of CLUE students indicate each IMF operates between molecules, when we look at consistency we see that a somewhat smaller group, 46% (N=40), receive "between" molecules codes for all three IMFs representations. In the traditional student population only *one* student out of the entire sample consistently represented all three IMFs as occurring between molecules. Only 6% (N=5) of CLUE students consistently received within codes for all three IMFs representations, while a significant subset of traditional students consistently represent IMFs as interactions within a single molecule (38%, N=36) or provided an ambiguous representation (2%, N=2). This leaves a majority of traditional students (59%, N=55) who were inconsistent in their depictions of intermolecular forces as examples of the same phenomenon (be it within or between). Similarly, even though a majority of CLUE students provided accurate representations for the location of each IMF as between molecules, in fact many CLUE students (47%, N=41) were inconsistent from one IMF to another. All percentages of CLUE and traditional students' responses that consistently received the same drawing code are provided in Appendix M.

Study 2: Results and discussion – Michigan State University, Cohort 3, end of GC2

While we were able to successfully reproduce our initial findings of the impact of the CLUE curriculum on students' understanding of IMFs with a second cohort of students taught by a different instructor, it might be argued that the results are not generalizable since all of the responses collected from both CLUE and traditional students for the first study came from a single university. Therefore, we administered the IMFA to both CLUE and traditional students enrolled in a second-semester general chemistry course (GC2) at MSU. Figure 7.3 shows the CLUE students' performance on the IMFA from both cohorts at Clemson (Univ. 1) as well as the third cohort from MSU (Univ. 2).



Figure 7.3: Code frequencies for CLUE students' drawings of all three IMFs from all three cohorts collected at two universities

As shown in Figure 7.3, the CLUE students' responses are quite consistent among the three cohorts. However, we cannot make statistical comparisons between them because we do not have measures for student performance or prior achievement that are consistent across all three cohorts. For hydrogen bonding, slightly more than 80% of students in all three cohorts received between codes for their representations. Between 58% and 72% of students in each cohort received between codes for their drawings of dipole-dipole and LDFs. It is notable that these responses are similar despite the differences in classroom environments between Clemson and MSU.

We also collected IMFA responses from students enrolled in the traditional course at MSU. The data were collected in the same manner as the CLUE student responses, and the students were given the same amount of credit for completion of the activity. While we cannot make claims about any comparison between CLUE and traditional student achievement since the
students were not a matched cohort, we did find that traditional students at MSU had great difficulty with this task as seen below. Figure 7.4 shows code frequencies for traditional students' responses from Clemson, (as shown earlier) along with the results from traditional students at MSU. The percentage of students from MSU who drew IMFs between molecules was similar to traditional students from Clemson (23% (N=56)). However, when compared to Clemson, far fewer students from MSU provided representations of IMFs within molecules. Instead, as can been seen from Figure 7.4, larger percentages of students at MSU (Univ. 2) received other codes which include "ambiguous", "not present", and "student DK" codes. A larger percentage of students at MSU (24%, N=57) had difficulty drawing the structure of ethanol for the IMFA than at Clemson (13%, N=12), which also made it difficult to interpret some of their representations and determine the intended location of each IMF. Additional graphs showing the frequency of all other codes can be found Appendix N.



Figure 7.4: Code frequencies for traditional students' drawings of all three IMFs from all three cohorts collected at two universities

Study 3: Longitudinal study results and discussion – Clemson, Cohort 1, GC2 through OC2

As noted in the DBER report⁷, longitudinal studies of student learning are rare for many reasons. They are often difficult, expensive and time-consuming, and it is frequently impossible to track students over time because of the varying paths they take through their studies. We were able to follow a group of students from Cohort 1, both CLUE and traditional, through a full year of organic chemistry. Organic chemistry, however, is not required for all majors and, as might be expected, there was a significant reduction in our sample size. By the end of OC2, 25 traditional students and 30 CLUE students remained from the original Cohort 1 who had completed all administrations of the IMFA over the course of two years.

A comparison of the two groups showed that, even after a full year of organic chemistry, the majority of CLUE students continued to show IMFs between molecules and the traditional students still represented IMFs as occurring within molecules, as seen in Figure 7.5. That is, there was very little change in the students' representations of all three IMFs once the students left GC2. Statistical comparisons between CLUE and traditional groups at each time point (the end of GC2 and again at the end of OC2) are shown in Table 7.4. The significant differences that were present at the end of GC2 were still significant after a full year of organic chemistry instruction with medium to large effect sizes.



Figure 7.5: Longitudinal comparison of CLUE and Traditional students' code frequencies for representations of hydrogen bonding, dipole-dipole, and LDFs from GC2 to OC2 (Cohort 1)

Table 7.4: Statistical results for longitudinal comparison of code frequencies for CLUE and Traditional students' hydrogen bonding drawings. p-values from chi-square analysis are provided with calculated effect sizes (ϕ , phi coefficient)

Drawing	Semester	Code	Traditional percentage	CLUE percentage	p-value	φ
Hydrogen bonding	GC2	Within	72	10	<.001	0.60
		Between	24	90	< .001	0.63
	OC2	Within	64	3	< .001	0.61
		Between	36	90	< .001	0.53
Dipole- dipole	GC2	Within	56	7	< .001	0.50
		Between	20	87	<.001	0.63
	OC2	Within	60	0	<.001	0.63
		Between	8	70	.001	0.45
LDFs	GC2	Within	60	10	<.001	0.49
		Between	8	70	<.001	0.59
	OC2	Within	60	3	<.001	0.58
		Between	20	77	.001	0.53

Figure 7.6 shows a Sankey diagram of Cohort 1 students' hydrogen bonding responses over time, and again it is clear that there is very little change in student responses after they leave GC2.



Figure 7.6: Code frequencies applied to Cohort 1 CLUE and traditional students' representations of hydrogen bonding at the end of GC2 and again at the end of OC2

While the sample sizes are small, it seems clear that neither group changes much over an entire year of organic chemistry. While this is evidence that the effects of the CLUE curriculum are not temporary, it does show that organic chemistry does not seem to improve traditional students understanding of IMFs. This is not particularly surprising since most organic faculty presumably believe that students have already learned this material in general chemistry (despite the fact that a robust understanding of organic chemistry requires students to understand how molecules interact as a prelude to reactions). What our study implies is that the understanding of IMFs that students develop in general chemistry is crucial.

Conclusions

As discussed earlier, the CLUE curriculum is explicitly designed to help students build a strong foundation of core ideas using a scaffolded progression of concepts. The topic of IMFs is central to a robust understanding of structure-property relationships. Not only do students need to understand the linked set of ideas that support understanding of IMFs, but they also must understand the subsequent role of IMFs in a wide range of chemical phenomena including phase changes and chemical reactions. In the CLUE curriculum, students are required to construct and revise answers to questions on a daily basis, whereas the traditional general chemistry course, like most general chemistry courses, covers the material following the order of topics in the textbook. However, as with most general chemistry curricula, the design of the traditional course does not explicitly connect the numerous steps required to connect structure and properties, in which an understanding of IMFs plays a significant part, and little focus is placed on scaffolding these topics and building upon earlier foundational ideas. To understand IMFs, students must be able to use the molecular structure to predict the molecular polarity and must also understand how the interactions between molecules determine properties such as melting or boiling points and acid-base behavior. If these ideas are not explicitly connected and reinforced at each step, and if students do not understand how each idea relates to the others and is used, then we believe students may not learn the material meaningfully and will instead rely on heuristics and rules.14,45-47

Limitations

The limitations of this study are twofold. First, we only have data from two universities. It will be important to determine if a wider range of students have the same kinds of trouble constructing representations of intermolecular forces and whether the CLUE curriculum is as effective when more broadly disseminated. We also do not discuss here whether students can actually put their understanding of IMFs to use; that is, can they use IMFs to predict relative melting and boiling points and to explain how molecules interact? These studies are ongoing and will be reported elsewhere.

Implications for teaching

We believe that the results shown here stem directly from the carefully designed CLUE curriculum, where the important concepts are connected, and students are made explicitly aware of the purpose of each of the concepts and skills being learned. That is, students learn meaningfully in ways that allow them to put knowledge to use. In addition, students regularly construct and use chemical representations to explain and predict phenomena. We believe that the inability of many students at MSU to construct reasonable drawings of individual molecules is a consequence of the fact that they were never asked to construct answers to prompts, but rather they practiced multiple-choice questions that test fragments of knowledge and recognition.

In this study, students do not appear to change they way they think about intermolecular forces once they leave general chemistry. Clearly this is problematic, both for future studies in chemistry, but also in biology where an understanding of IMFs (and more broadly non-covalent interactions) is assumed as prior knowledge. If the majority of students have (at best) an inconsistent notion of this concept, it is unlikely that they will be able to reason about molecular interactions appropriately.

While there are certainly many ways to improve student understanding (besides wholesale adoption of a new curriculum), we believe that, at the very least, students must be asked to construct representations and to draw and write about their understanding of chemical principles. It is also important that students be made explicitly aware of the purpose of the fragments of knowledge and skills that they are learning and that instructors help them to construct a more coherent base of knowledge on which to build their future understanding. REFERENCES

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CHAPTER 8: AUTOMATED LEXICAL ANALYSIS OF STUDENTS' DESCRIPTIONS OF HYDROGEN BONDING

The key idea to keep in mind is that the true power of educational technology comes not from replicating things that can be done in other ways, but when it is used to do things that couldn't be done without it. - D. Thornburg¹

Introduction

The NRC's recent framework for science education has outlined the need to incorporate scientific practices, disciplinary core ideas, and cross-cutting concepts into STEM courses.² While these changes are crucial to improving the way STEM content is taught, in order to successfully incorporate these changes we have to reconsider the ways in which we assess student knowledge. Specifically, we need to ensure that we are creating meaningful assessments that target key ideas and practices. Today, multiple-choice (or forced-choice) assessments are an extremely common form of testing in post-secondary education. Multiple-choice (MC) assessments certainly have their benefits, which undoubtedly have contributed to their rising popularity over time. They are easy to administer to large groups of students and typically result in quick and consistent scoring.³ In fact, Zeidner found that most students prefer multiple-choice over essay exams because they often view them as easier, less complicated, and less stressful. Oddly enough, this is despite the finding that the majority of students found it easier to prepare for MC exams, spending less time and effort studying.⁴

There are certainly disadvantages to using MC assessments to elicit student

understanding. By design, multiple-choice questions limit the number of possible answer choices a student can make; they can also provide unintended benefits for students like allowing students to work backwards from provided answers and increasing the odds of students guessing the correct answer.⁵ Effective MC questions can be difficult to design and poor distractor choices can inadvertently lead a student to the correct answer. Additionally, Birenbaum and Tatsuoka compared the effect of multiple-choice and open-ended test formats on students' ability to solve fractional addition problems and found it more difficult to identify students' underlying misconceptions using multiple-choice items when compared to an open-ended format.⁶

As shown from our own interviews, students are certainly able to circumvent the intent of questions like boiling point ranking tasks by memorizing general trends or rules rather than using a deeper understanding of the relationship between structure and properties.⁷ Fisher and Lipson suggested that, "humans exhibit a fairly strong tendency to avoid extra mental effort, so as to minimize their information processing load and to conserve their attentional resources. This tendency often results in attention to, and use of, superficial rather than deep-structure aspects of a situation."⁸ The propensity to use heuristics, memorization, and trends is well documented in the chemistry education literature and is not particularly surprising.^{7,9–12} Heuristics and trends allow us to bypass our deeper System 2 thinking processes in favor of the faster and more efficient System 1 processes.^{13–15} While heuristics and shortcuts certainly have their benefits when used appropriately, much of chemistry (and STEM disciplines in general), require the conscious use of System 2 processes to truly develop understanding of the subject matter. Assessment questions that promote deeper thinking are certainly more favorable for probing student understanding of scientific concepts. While some MC questions could be constructed in

such a way as to get at this understanding, there are other question formats that may be better suited for uncovering students' understanding.

Constructed response questions include a wide range of question formats ranging from free-response and essays to drawings and graphs.¹⁶ Unlike their multiple-choice counterparts, they often cover greater cognitive range and can elicit complex performance and divergent student ideas.¹⁷ Drawings in particular can provide a unique view into student understanding and can help foster a deeper learning of science.^{18–22} Several studies have compared responses from students who wrote explanations to those who provided drawings, and they found differences in the features emphasized by each group.^{23,24} Indeed in our own work described in Chapter 6, we were better able to determine spatial information from students' drawings; often, spatial information was omitted from students' written responses entirely.²⁵ By requiring students to draw representations, we can get a glimpse into the ways in which they think about chemistry on the microscopic and particulate levels.^{18,20,26} While requiring students to construct representations can certainly be illuminating, it is not always practical. Viewing and scoring large numbers of student drawings can be time consuming and requires a well-defined and refined scoring rubric. In order to use these rubrics graders require training and calibration; even so, the scoring of responses is not always consistent.

Open-ended written explanation questions provide a middle ground between MC questions and those requiring students to construct representations or graphs. Like drawings, students' written responses allow for greater variety. As Ha and colleagues outlined in their own studies in the field of biology, most MC assessments focus on identifying either novice or expert ideas. Many do not allow for the wide range of interconnected ideas that students often possess.²⁷ Indeed, diSessa's theory of phenomenological primitives supports the notion that students

possess a large and varied set of fragmented ideas that can be combined in different ways to inform their understanding of a phenomenon.²⁸ Open-ended writing formats are better able than MC questions to reveal the assortment of ideas that students possess and how they are interwoven.²⁷ Sadly, these questions possess similar drawbacks to drawing and constructed responses. Specifically, they can be difficult to interpret, require more time to score, involve extensive grader training, and have greater variability in rater scoring.²⁹ While constructed representations can provide some additional benefits over open-ended writing questions, like eliciting structural information^{23–25}, the scoring of students' written responses has seen sizeable technological advancements in recent years. Researchers are now training computer programs to code text responses like discipline experts.

Automated computer scoring

Automated computer scoring allows researchers to train computers to predict human scoring of written responses using a series of algorithmic models. This is often achieved through a standard procedure. Human researchers code (or score) a large set of written responses. Typically, this larger set of responses is then divided into two smaller sets: a training set and a validation set. Computers use the training set to create algorithms and models that best fit the data provided. These algorithms can then be applied to the validation set and the resulting scoring predicted by the computer is compared to the original human scoring. If the models and algorithms are robust, there should be high agreement between the computer scoring and human scoring.³⁰ Many studies have successfully used automated text analysis, or lexical analysis, to achieve high scoring agreement for written essays and short answer responses.^{27,29–33} Several studies in the field of biology education specifically, ranging from evolution to acid-base

reactions, have found computer scoring models to accurately reflect human scoring.^{27,29,32} A well-designed and tested automated scoring model should ultimately provide quick, uniform coding of students' responses. Other additional benefits of automated analysis include the fact that computers lack bias, do not grow tired of coding, and are consistent in their scoring (unlike humans at times).³⁰

While there are numerous programs^{34–36} available for text analysis, we used SPSS Modeler, a commercial software program provided by IBM, to conduct our text analysis.³⁷ SPSS Modeler includes a wide range of predictive analytic tools, including text analytics, to inform and guide research. After importing large sets of text data, Modeler identifies, as best it can, every term used in the provided responses. The program comes with a library of preset dictionaries that include common terms the system readily recognizes. The user can add new terms to an existing dictionary or create new dictionaries to expand the terms the software can recognize, like creating a dictionary for terms related specifically to chemistry. Once the software recognizes the relevant terms, it is the job of the researcher (or user) to place the important and relevant terms into appropriate bins, or categories, for later analysis. For instance, the researcher would combine terms like "proton" and "H+" into one category labeled Hydrogen *Ions.* Once categories have been established, Modeler offers an array of statistical tests that use these categories as variables in exploratory or predictive statistical models. Exploratory statistical tools allow researchers to visualize connections between categories or cluster similar responses together. Predictive statistical models result in a "scoring" algorithm to predict a human expert score, which allows the researcher to compare Modeler's application of categories against an expert's coding scheme.

Text analysis, with programs like Modeler, has some disadvantages. For instance, in order to build a robust model, the system typically requires a large number of text responses to analyze (on the order of hundreds). An additional set of responses, preferably large in size, is required to test the created model for validity. However, large data sets are not the only downside. Certain question formats, such as compare and contrast questions, often do not perform well in Modeler, at least not without extra work on behalf of the user. So, for example, when students compare and contrast an acid and a base, they often (and should) discuss both types of compounds. However, because the system does not have a built-in proximity function, it cannot determine if words such as acid or base go with sodium hydroxide or with hydrochloric acid. The system can identify that a student used both compound names but cannot determine which words in their response relate to the acid and which relate to the base.

While the use of SPSS Modeler does require a large amount of work in the initial phases, the rewards of creating a robust set of categories and predictive models can be numerous. For instance, once a successful model is built that achieves high agreement with an expert's codes, new sets of text responses can be inserted into the model to be automatically scored. This is particularly useful when analyzing student responses across multiple courses or years. For example, if an instructor were interested in giving the same question each year to monitor the progress of a specific group of students, they could potentially use a single model to continually and consistently analyze new responses.

Purpose of study

With our previous studies, we attempted to explore the connection between what students say and what they draw. That is, do the constructed representations they provide for IMFs align

with the ways in which they describe IMFs? We found that students were more likely to provide structural information, like the location of IMFs, in their drawings than in their written description of IMFs. Because of this, location codes assigned to students' text and drawings often did not align. We were interested to see if automated text analysis of students' written descriptions of IMFs could predict the code assigned to their drawings of IMFs. That is, since our hand coding of students' text responses only addressed the location of IMFs, we wanted to know which words or combinations of words were more strongly associated with students who represented IMFs as *between* molecules rather than within. Coding drawing responses is certainly time-consuming, and a successful predictive model for students' drawings based off of their text responses could provide quick feedback as to their level of understanding.

For this analysis we chose to explore students' descriptions of hydrogen bonding as compared to their drawings of hydrogen bonding as elicited on the IMFA. By doing so, the content of both questions is the same with the difference lying in modality. Specifically we were interested in the following research questions:

RQ1. How well does lexical analysis of students' written description of hydrogen bonding predict the location of hydrogen bonding in their constructed representation?

RQ2. What impact does an alternative general chemistry curriculum have on students' written IMFA responses? That is, can lexical analysis of written responses differentiate between students enrolled in different curricula?

Methods

Data for this study was collected from students enrolled in the second-semester of general chemistry at Michigan State University (MSU, Cohort 3). These are the same CLUE and traditional student responses analyzed in Chapter 7 to compare the performances of students on the IMFA across different universities and curricula. For this particular study, we chose to use data from MSU because of the need for a large number of responses (N=320). While we could have combined responses from both Clemson and MSU to create a larger student sample, there is some evidence that the university at which students are enrolled can affect the language of their responses and thus the outcome of text analysis.²⁷ In order to reduce the number of possible confounding variables, we limited responses in our study to those from a single university, collected at a single time point. We did, however, include both CLUE and traditional general chemistry students' responses in this study. We did not have enough responses from the traditional group (N=144) or CLUE group (N=176) alone to create reliable statistical models.

For analysis, we used students' responses to items 2, 4, and 7 of the IMFA, outlined previously in Chapter 5. Text responses from items 2 and 4 were exported from beSocratic, combined, and imported into SPSS Modeler. To produce reliable results, automated computer scoring requires a sizeable sample of responses for each drawing code from item 7 from which a model is built. Therefore, the only drawing codes models we report in this analysis are "between" and "within" as all other drawing codes had extremely small sample sizes (less than 40 responses). With such a small number of responses, we could make some claims based on the results, but more responses would certainly be needed to verify the validity of any findings. For our two main drawing codes, 67 students received a "within" code and 196 students received a "between" code.

Lexical category creation

After we uploaded our entire data set of 320 responses into Modeler, the text analytics package extracted 263 "concepts" (or words) as seen in Figure 8.1(a). From these "concepts", we created 59 fine-grained lexical categories (LC). That is, most categories we created were for a single word/term, like "nitrogen", and were pertinent to the topic of hydrogen bonding. We did not make categories for words like "one" or "not applicable" that may have been prominent in our data but alone, held little meaning or more than one meaning, making them difficult to correctly and reliably categorize.

Examples of created categories can be seen in Figure 8.1(b). The *Fluorine* lexical category, for example, consisted of terms like "F", "flourine", and "florine". It also included terms such as "onf", which students often used as a substitution for writing out "oxygen, nitrogen, and fluorine". This term and others like it were also included in both the *Oxygen* and *Nitrogen* LC's for consistency. An example of LC application can be seen for Jordan's response, "Hydrogen bonds are weak attraction forces between hydrogen and another atom because of hydrogens partial positive charge." Jordan's response would be categorized as *hydrogen bond, strength, attraction* (as a subcategory of interaction), *force, between, hydrogen, another, atom,* and *polarity* (specifically the subcategories partial, positive, and charge). It was extremely common for an individual response to be classified in several different categories. These connections between multiple categories can distinguish between groups of responses during later statistical analysis.

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hydrogen	(362 (10%)	290 (91%)	🗔 <mwunique></mwunique>
hbnd	🝵 fx	254 (7%)	232 (73%)	🗔 <type 1=""></type>
bond	fx	217 (6%)	173 (54%)	园 <type 1=""></type>
between	🝵 fx	177 (5%)	161 (50%)	厉미 <type 1=""></type>
atom	6	185 (5%)	128 (40%)	5리 <type 1=""></type>
molecule	∱ [™] fx	176 (5%)	121 (38%)	厉리 <type 1=""></type>
another	🗎 fx	93 (3%)	81 (25%)	厉리 <type 1=""></type>
not applicable		75 (2%)	75 (23%)	🖼 <uncertain></uncertain>
strong	(82 (2%)	74 (23%)	园 <kchunique></kchunique>
oxygen	6	80 (2%)	73 (23%)	园 <lc_old></lc_old>
electronegative	6	79 (2%)	59 (18%)	🖼 <unknown></unknown>
nitrogen	6	60 (2%)	58 (18%)	🖼 <unknown></unknown>
s f	<u> </u>	53 (2%)	51 (16%)	厉리 <type 1=""></type>
s element	6	59 (2%)	50 (16%)	🗔 <type 1=""></type>
0	6	50 (1%)	46 (14%)	🖾 <metabolismcommon></metabolismcommon>
n	6	46 (1%)	44 (14%)	🗔 <type 1=""></type>
🔪 fluorine	6	39 (1%)	38 (12%)	🖼 <unknown></unknown>

Category Descriptors Docs ⊽ Image: All Documents - - Image: Uncategorized - - Image: No concepts extracted - - Image:	20 4 2 0
■ All Documents - - Uncategorized - - No concepts extracted - ■ ⊕ Hydrogen 9	320 * 2 0 '94
Uncategorized - No concepts extracted - □- ⊕ Hydrogen 9	2 0 '94
No concepts extracted	0 '94
🖶 👚 Hydrogen 9	94
🖶 👚 H-bond 7	34
	80
🖶 😁 Between 3	63
	59
🖶 😁 Atom 2	28
👜 🝵 Molecule 9	25
🖶 😁 Interaction 17	94
👜 😁 Strong 6	86
🖶 😁 Another 1	81
👜 🝵 Electronegativity 16	74
🖶 😁 Polarity 40	71
🖶 🝵 Between molecules 2	68
🖶 😁 Element 1	50

(b)

Figure 8.1: a) Examples of terms (concepts) extracted by Modeler using the Text analysis node; b) Examples of lexical categories created for terms extracted by Modeler

Some of our more complex lexical categories arose from a need to address differentiation in word use. For instance, the term "bond" when used generally does not have the same meaning as "bond" contained in the phrase hydrogen bond. Unfortunately for us, Modeler recognized "hydrogen bond" not as a scientifically distinct term, but as simply "hydrogen" and "bond". Unlike some text analysis software packages, Modeler does not have a built-in word proximity function that would allow us to consider "bond" as a different term when it is within a certain proximity of "hydrogen". Because of this, our initial attempts to capture bond separate from hydrogen bond were unsuccessful. Our solution involved creating an entirely new term in the chemistry library within Modeler ("hbnd") and linking this software term with the word(s) hydrogen and bonding in student responses. This allowed the software to differentiate between bonds used in the general sense ("bond"=bond) and the specific sense (hydrogen bond = "hbnd"). We used a similar solution to address the difference between the term "force" and London dispersion forces by creating the term "LDFs". We were able to use rules functions within Modeler to create LC's for groups of words. For example, we created the *Between Molecules* LC to attempt to identify the location of the IMF that students were describing. The goal of this rules-based LC was to distinguish between students using the term "between" to refer to between atoms or specific elements instead of between molecules.

We also created a few "larger" categories by combining related subcategories. For instance, we created a *Correct EN Atoms LC* that included the terms "oxygen", "nitrogen", and "fluorine". We decided to combine these categories after a cursory cluster analysis revealed that students most often used these three terms simultaneously. Conceptually, we were not particularly concerned if students could remember all three electronegative atoms involved in hydrogen bonding. In the same manner, we created the *Polarity LC*, which contained terms like "dipole" (not to be confused with dipole-dipole) and charges, and the *Incorrect EN atoms LC* with terms like "carbon" and "sulfur". For analysis purposes, we could choose to treat these either as large categories or split them out in to their individual subcategories if we wanted a more detailed analysis.

It is important to note that, while Modeler is particularly good at extracting terms from a given set of responses, it cannot assign meaning to these terms. That is, Modeler can identify the

term "bond" and "force" for a student response, but it cannot identify the underlying meaning of a phrase such as Sarah's, "creating an attractive force between the two but a hydrogen bond is not actually a real bond." This means that Modeler would apply the *Force LC* and *Bond LC* to Sarah's response despite the fact that she uses the word bond to describe hydrogen bonding as **not** a bond. Unfortunately, there are not many simple ways to correct for this error. The most obvious solution is the inclusion of a proximity function, which Modeler does not have. For our data, responses like Sarah's were uncommon, and we decided to leave the *Bond LC* as is, even though a few responses would get incorrectly categorized. Ideally, the categorization of the rest of Sarah's response, and the responses of those like hers, would play a larger role in her classification via discriminant analysis than a single misapplied category.

Applying discriminant analysis

We used the discriminant analysis function in Modeler to determine if students' text responses about hydrogen bonding could be used to predict the location code they would receive for their subsequent drawing of hydrogen bonding. Discriminant analysis works by creating a discriminant score for each text response from a number of independent variables. In this case, our independent variables were the LC's that we created. These discriminant scores can often be combined into groups based on similarity of scores, creating a mean discriminant score called the group centroid. Discriminant analysis attempts to maximize the distance between group centroids to create higher performing models. These discriminant scores can then be used to predict the probability that a specific response falls into a given dependent variable category (in our case whether or not a student draws hydrogen bonding as occurring between molecules). The larger

the difference between the centroids, the more distinctive the groups are and the better the model will perform in predicting which responses fall into which groups.³⁸

We chose discriminant analysis over linear regression since discriminant analysis is better suited for categorical data, such as our mutually exclusive drawing codes. Additionally, discriminant analysis measures how the independent variables change together (the covariance).³⁸ Because of this, the interactions between the LC's play an important role in the analysis. We chose to use a step-wise discriminant analysis in Modeler. By doing so, Modeler works to build a model by adding categories one at a time until the model no longer shows improvement. This helps to prevent over-fitting the model, which is especially important when working with smaller sets of data.

Categorizing responses using web diagrams

While discriminant analysis can be useful in predicting the coding category a response would receive, it can be a complicated process if the goal is to generally characterize a group of responses. Since our data set consisted of responses from both CLUE and traditional students, we chose to use web diagrams to explore similarities and differences in students' text responses from these two groups. While we knew from previous studies that these two groups differ in both how they represented IMFs and whether they discussed the location of IMFs in the written descriptions, we were also interested in exploring what other differences might exist in the language they used to describe IMFs. Modeler provides the option of creating web diagrams to highlight terms that are often used together within students' responses. This can provide insight into connections students think are important in answering the question and characterize similarities and differences in the ways each group describes IMFs.

Web diagrams show which LC's (selected by the researcher) are more commonly used together in students' text responses. Using too many LC's can make the web diagram difficult to interpret, so care must be taken when selecting categories to include. LC's are represented in the web diagram as nodes with lines (or links) of varying thickness connecting them to other LC's. These links represent a connection between two LC's, meaning both LC's were used in a given number of responses. The thickness of the line relates to the prominence of the link in terms of overall percentage. For example, a link between *Hydrogen* and *Acid* with medium thickness could represent 10% of the number of overall links made. Differences in the type and thickness of various links can help characterize differences in how our two groups discuss hydrogen bonding.

Results and Discussion

Using discriminant analysis with lexical categories to predict the hydrogen bonding drawing code

Of the 59 LC's we created, the most prominent categories assigned to the data set were *Hydrogen* followed by *Hydrogen Bonding* and *Bond*, as seen in Table 8.1. This is probably because students often repeat words given in the prompt (like hydrogen bonding) in their responses. Perhaps more interestingly, words that we would hope to see in students' responses, like molecule, interaction, and another, were used by less than half of the sample. Additionally, there is an interesting difference in the percentage of responses that fall in the *Between LC* as opposed to the *Between Molecules LC*. While the word "between" is a term that ideally should be included in students' responses, the word alone is not always indicative of between molecules.

Note that about half of the students used the word "between", but only approximately 20% of

students use the word to describe the relationship between molecules.

Lexical category	Percent of responses with the
	lexical category
Hydrogen	91.9%
Hydrogen bond(ing)	73.1%
Bond	56.3%
Between	50.9%
Correct electronegative atoms (includes O, N, and/or F)	49.7%
Atom	40.0%
Molecule	39.1%
Interaction	29.3%
Strong	26.9%
Another	25.3%
Electronegativity	23.1%
Polarity (includes dipole, charges, negative, and positive)	22.2%
Between molecules (category using rules to collect responses using between and molecules)	21.3%

Table 8.1: Most commonly assigned lexical categories (those applied to greater than 20% of the total sample)

In order to address our first research question, we used discriminant analysis to develop models that could predict the drawing code a student would receive for their constructed representation using their written description of hydrogen bonding. We generated two independent models, one for each drawing code (between and within) using the entire data set (N=320). Table 8.2, shown below, lists the lexical categories chosen by Modeler as predictors for each model. For the model that predicts the "Between" molecules code, Modeler selected a total of fourteen LC's to use as predictors variables; each variable has it's own coefficient which shows that particular variable's contribution to the scoring function (similar to beta-weights in a regression analysis).³⁸ The variety of LC's used by the model shows that, rather than a single term that easily discriminates, it is a combination of all of these terms that distinguishes between students' responses.

The model for the "Between" molecules code accounts for 32.5% of the variance (Wilks' lambda = 0.675, chi-square = 122.082, degrees of freedom = 14, p-value = <0.001) and the significant p-value leads us to believe that there is a relationship between the "between" molecules drawing code and our LC's. The association of positive and negative predictor values listed in Table 8.2 is dependent on where Modeler places the group centroids. In each model, there are only two groups: presence or absence of the drawing code. It's easiest to think of centroids as being placed on a linear axis, ranging from negative to positive values.³⁸ For example, for the between model, the system placed the group centroid for responses that received a between code (present) at 0.550, while placing the centroid for those that did not receive a between code (absent) at -0.869. For this particular model, coefficients with a positive value are more likely to cause a response to be predicted to have a present between code rather than the absence of the code. Of the fourteen variables selected by Modeler, nine had positive coefficient values indicating they were more strongly associated with receiving a between drawing code; the largest coefficient was associated with the LC Oxygen. When considering the context of the question, these nine lexical categories make sense. We would associate LC's like Molecule and Another with the understanding that hydrogen bonding is an interaction between molecules. Additionally, the inclusion of the LC's *Electronegativity* and *Polarity*, which are more closely associated with understanding of scientific principles, also lend to a more developed understanding of IMFs as interactions. This means that students who included ideas like electronegativity, polarity, and interaction in their writing were more likely to receive a between molecules code for their drawing.

Model	I C nomo	Canonical
Widdei		coefficients
	Oxygen	0.549
Between	Electronegativity	0.431
	Molecule	0.363
	Polarity	0.337
	Another	0.323
	Different	0.228
	Interaction	0.175
	IMFs	0.103
	Electrons	0.091
	Attached	-0.030
	Occur	-0.036
	Atom	-0.114
	Bond	-0.156
	Carbon	-0.262
Within	Molecule	0.659
	Electronegativity	0.403
	Negative	0.383
	Bond	-0.396

 Table 8.2: Lexical categories used as standardized canonical discriminant function coefficients

 for each drawing code model

Similarly, five categories were listed as negative predictors for the "between" molecules model, and the larger negative values make sense as predictors for the lack of a between molecules code in the context of the assessment. We would hope that students who possess a strong understanding of hydrogen bonding as an interaction between molecules are less likely to include terms like "bond" and "carbon" in their written descriptions. Unlike nitrogen, oxygen, and fluorine, carbon does not participate in hydrogen bonding because the electronegativity difference between carbon and hydrogen is relatively small (or practically negligible), so students should not be discussing carbon as part of their explanation of hydrogen bonding. Student text responses that discussed terms like "carbon" and "bond" were more likely to not receive a between molecules drawing code (absent). It is important to note that the *Bond LC* included here encompasses students' general use of the term "bond" while omitting bond in the context of hydrogen bond(ing). While there are a few scenarios in which a student may appropriately include the term bond while discussing hydrogen bonding (like Allison describing it as "when a hydrogen that is bonded to an atom like oxygen or nitrogen is attracted to another atom with a high electronegativity") responses like Allison's are considerably less common than the inappropriate application of the term "bond".

Conversely, only four lexical categories were used by Modeler to create a model for predicting the "within" drawing code (Wilks' lambda = 0.893, chi-square = 35.758, degrees of freedom = 4, p-value = <0.001). Unlike the between model, the group centroid for the presence of a within code was negative while the absence of the code was positive. This means that the lexical category *Bond* was the only predictor used in the computer model for those who received a within drawing code. *Electronegativity*, *Molecule*, and *Negative* were used as predictors for absence of the within drawing code. For students who represent hydrogen bonding as a covalent bond within the molecule, it makes sense that their discussion of the IMF would also include the term "bond". Additionally, it is understandable that their explanations would lack the inclusion of terms related to scientific principles.

Both models created were moderately successful in predicting students' drawing codes. Specifically, the between model correctly classified 78.1% of students' responses and the within model correctly classified 79.1%. Modeler provides a break down of responses into correct classifications, false positive, and false negatives. Correctly classified for our study meant that the predicted presence or absence of a drawing code from our model matched the human scoring of a student's drawing. Table 8.3 shows the classification break down both drawing code models. With this information we can see where our models may be lacking and attempt to refine them.

Lexical category	Correctly classified	False negative	False positive	Cohen's kappa
Between	250 (78.1%)	31 (9.7%)	39 (12.2%)	0.54
Within	253 (79.1%)	67 (20.9%)	0 (0%)	N/A

Table 8.3: Agreement and classifications of the between and within drawing code models

Using the information in Table 8.3, we can calculate Cohen's kappa for the between and within drawing codes. Even though the percent agreement between the human coder and Modeler is fairly high, calculating inter-rater reliability allows us to factor in the effect of chance agreement between raters. We could not calculate kappa for the within code because Modeler did not predict any student responses as having a within code, resulting in no false positives. As a result, it is difficult to make any inferences about reliability for the within code. For the between drawing code, we calculated a Cohen's kappa of 0.54. Typically, kappa values from 0.4-0.6 are considered moderate and 0.2-0.4 fair.³⁹ These kappa values, however, are lower than we would normally expect for inter-rater agreement. Often, we report values at 0.8 or higher when comparing the scoring of two human coders. While the percentage of correctly classified responses for the between model (78.1%) and the within model (79.1%) aren't as high as we had hoped, we have to consider the fact that we are trying to use students' written responses to predict their performance on a drawing task. Typically, discriminant analysis is used to predict human scoring of written responses. Considering the fact that we are attempting to use student writing to predict student drawings, we consider the percentage of students correctly classified by the "between" model to be moderately successful.

Exploring differences in CLUE and traditional student responses using web diagrams

In order to address our second research question, we chose an exploratory approach to identifying the differences between students enrolled in the CLUE and traditional curricula.

Rather than starting with discriminant analysis, we chose to explore the links between LC's for each group (CLUE N=176, Traditional N=144) using web diagrams. It is important to note that Modeler's web diagrams identify two LC's as linked if both appear in a single response. This does not necessarily mean that students' have explicitly or correctly connected these ideas in their response, only that the terms or concepts appear together. We selected LC's with strong correlations to our CLUE/traditional course variable to observe how students were connecting these terms and with what prevalence. For instance, do some students more readily use both bond and oxygen in their response, and what inferences can we make from that information? For creating web diagrams of CLUE and traditional student responses from MSU, we included the following lexical categories: Another, Bond, Carbon, Correct Electronegative Atom, Dipole-Dipole, Element, Hydrogen Bond(ing), Highly, Hydrogen, Intermolecular Forces, Lone (specifically in reference to lone pair), Molecule, Not, Polarity, Weak, Interaction, Occur, and Present. Subcategories for the LC's Interaction and Polarity were subsumed under the main category for simplicity as fewer categories typically lend to web diagrams with greater readability. The only exception was for the Correct EN atoms LC where the subcategories Oxygen, Nitrogen, and Fluorine were individually included.

For the web diagrams included here, we chose to have the lines between categories represent overall percentages. By using overall percentages, we can show values as percentages of the total number of links in the web diagram. For instance, 2.6% of links made by CLUE students were between hydrogen and oxygen. It was the fourth highest percentage out of all links made by CLUE students. While 2.6% does not appear to be very large, we have to consider that, in total, CLUE students made approximately 3360 links. In absolute numbers, that means 88 CLUE students (or 50% of our sample) included both of these terms in their responses. By using

overall percentage, we can help reduce the impact of the fact that one group of students may simply write more than another group. In this way, if one group used the word "acid" more, but also wrote more words in general, the overall percentages between the two groups would be comparable and not skewed in favor of the group who simply wrote more words.

The web diagrams provided below only show percentages greater than 1% of the overall number of links for each group. Link percentages below 1% tend to apply to less than 10% of students in the sample and are often not as useful. Thicker lines denote stronger connections with link percentages greater than or equal to 2%, while thin lines show weaker connections with link percentages that fall between 1% and 2%. It's also important to note that the web diagram for traditional students contains two additional categories: *Carbon* and *Element*. These two lexical categories fell over the 1% threshold for traditional responses but not for CLUE responses. We will explore this more later, particularly in reference to carbon.

We can make some initial inferences from the web diagrams shown in Figures 8.2 and 8.3. While traditional students have more strong connections in general than CLUE students (16 compared to 13), CLUE students have more connections to LC's like *Polarity*, *Interaction*, and *Another*, which relate to an understanding of the correct underlying chemical concepts. The presence of the *Polarity LC* and *Interaction LC* again implies an understanding of the underlying scientific principles involved in interactions between molecules. The *Another LC* may be associated with the term "molecule" and most likely is in reference to the location of hydrogen bonding between molecules. While we did not require students to explicitly discuss the underlying causes of hydrogen bonding (i.e. columbic attractions between molecules arising from differences in electronegativity) it is interesting that more CLUE students are using these specific terms in conjunction with those common to all responses, such as hydrogen or molecule.



Figure 8.2: Web diagram of CLUE students' responses



Figure 8.3: Web diagram of traditional students' responses

As seen in Figure 8.3, traditional students made more connections with the LC's Carbon and *Element*. While the *Element* LC itself may not be particularly insightful, the addition of the *Carbon LC* is an interesting finding and is consistent with reports by Henderleiter and colleagues of students identifying carbon as capable of hydrogen bonding.⁴⁰ Generally, we do not expect students to discuss carbon when describing hydrogen bonding. Instead, both groups of students refer to specific elements like hydrogen, oxygen, nitrogen, and fluorine as is evident in both web diagrams above. It is important to note that the overall percentage is small for links to *Carbon*; the largest link is between *Carbon* and *Hydrogen* at 1.22%. Only about 10% of traditional students used the term "carbon" (compared to 2% of CLUE students). One way to correctly include carbon in a response would be to say that hydrogen bonding could not happen between hydrogen and carbon. However, we know that most, if not all, traditional students are not using the term "carbon" in conjunction with "not" due to the lack of a link in the web diagram. This allows us to infer that students are indeed indicating that carbon is capable of hydrogen bonding, and, after checking students' responses, we confirmed that none of the students used the term carbon to mean "not carbon". Therefore, the inclusion of carbon as an identifying factor of the traditional students is troubling.

We can glean other pieces of information from the data used to create the web diagrams. For instance, we know that CLUE students, in total, made an average of 3360 links while traditional students made about 1060 links. Taking into account their different population sizes, CLUE students made approximately twice as many links as traditional students (14 links per CLUE student and 7 links per traditional student). This indicates that CLUE students have longer and richer explanations. This is not entirely surprising considering that students enrolled in the traditional GC course at MSU are rarely asked to explain their understanding, unlike CLUE

students. Based on the web diagrams, the responses are not just longer, but contain more "correct"/valid chemistry concepts as well. While it's important to remember that these links apply only to the lexical categories we included for the creation of our web diagrams, these categories were specifically chosen because of their strong correlation to the CLUE/traditional variable.

Using discriminant analysis of student responses to predict GC course enrollment

After analysis of CLUE and traditional web diagrams, we used discriminant analysis to try and determine if Modeler could identify a student as CLUE or traditional based on their written response about hydrogen bonding. Using the lexical categories created from students' responses, we were able to successfully build a model to predict whether students from Cohort 3 were enrolled in the CLUE or traditional general chemistry course. In this case, only a single model (course enrollment) was necessary to determine if a student was in the CLUE or traditional group because these two groups were the only options for students in our data set. Our developed model had a Wilks' lambda value of 0.622 and a p-value of <.001 (chi-square = 148.852, degrees of freedom = 10), meaning the variables selected explained approximately 38% of the variation between the groups. As with our previous models used to predict students' drawing codes, our model achieved a fairly large separation between group centroids with CLUE at 0.704 and traditional at -0.860. With this in mind, Table 8.4 shows which LC's were most significant in discriminating between the two groups.

Model	LC names	Canonical coefficients
	Electronegativity	0.541
	Interaction	0.475
	Fluorine	0.389
	Bond	0.319
CLUE/traditional	Another	0.288
course	Element	0.271
	IMFs	0.242
	Oxygen	0.241
	Strength	0.207
	Carbon	-0.219

Table 8.4: Coefficients used in our model to predict students' enrollment in CLUE or traditional GC

Electronegativity, *Interaction*, and *Fluorine* had the highest positive function value indicating that they were stronger predictors for CLUE students. The LC *Interaction* is particularly encouraging to see listed as such an influential coefficient. As discussed previously, it is certainly preferable for students to refer to IMFs as interactions or attractions rather than bonds. The confusion of bonds and IMFs can result in other ideas, such as the notion that boiling breaks covalent bonds rather than overcoming IMFs.^{7,41,42} The inclusion of the LC *Electronegative* as a strong predictor of CLUE enrollment is also promising. While we did not specifically ask students why IMFs occur, the inclusion of a discussion of polarity and electronegativity alludes to a deeper understanding of the relevant scientific principles. Like CLUE students' stronger and more frequent links to the *Polarity LC* (as seen in the web diagrams), the inclusion of *Electronegativity* as a strong predictor is encouraging.

The *Fluorine LC* as the third highest predictor for CLUE enrollment was surprising. To the best of our knowledge, neither curriculum placed additional emphasis on fluorine as a requirement for hydrogen bonding (although it is one of the three elements most often cited). One possible reason for fluorine as a predictor of enrollment in the CLUE course is that the
CLUE curriculum's greater emphasis on polarity and electronegativity may result in more CLUE students' inclusion of fluorine in their explanations since fluorine is often noted as the most electronegative element, located at the top right of the periodic table. Additionally, we are unsure as to why the *Bond LC* was included as a predictor for CLUE enrollment. This category does not include hydrogen bonding, only the use of the term "bond" generally. It may be that CLUE students were referring to the need for hydrogen to be covalently bonded to oxygen, nitrogen, or fluorine in order to participate in hydrogen bonding.

Our predictive model for GC course enrollment performed slightly better than our previous models to predict a students' drawing code. The model achieved a percent agreement of 81.3% with a Cohen's kappa value of 0.622. These data along with false positives and negatives are provided below in Table 8.5. The kappa value for inter-rater reliability is just above the moderate threshold, classifying it as a "substantial" agreement.³⁹ While still not in our ideal range of higher than 0.8, again we want to emphasize the effect of the nature of the study on measurements of inter-rater reliability. As with our previous discriminant analysis models, we are attempting to use text responses to predict variables other than text coding or scoring rubrics. Additionally, we have only used one data collection to attempt to predict course enrollment. More responses from additional cohorts would most likely help highlight the differences between the courses. Like the drawing codes, when attempting to predict which course a student is enrolled in, we would not expect perfect agreement.

Table 8.5: Classification and agreement for the GC course model

9	<u> </u>			
Lexical category	Correctly classified	False negative	False positive	Cohen's kappa
CLUE/Traditional	260 (81.3%)	32 (10.0%)	28 (8.8%)	0.622

Conclusions

While our results using discriminant analysis of students' text responses to predict the location of IMFs in their constructed representations do seem promising, currently the models created are not robust enough to consistently and accurately predict drawing codes. While we did manage to achieve relatively high percentages of correctly classified responses, our models did not achieve large kappa values indicating less than ideal agreement between human coders and the predicted scoring. There are certainly several reasons as to why this may be the case. The model created for the within drawing code was heavily biased towards the presence of a within code, resulting in no responses being categorized as lacking a within code by Modeler. Some of these issues could possibly be mediated by using larger sample sizes. In fact, Ha and colleagues tested the effects of using a larger training set on automated computer scoring models with the machine-learning program LightSIDE⁴³, designed by LightSide Labs. They found that, by doubling the number of responses used to create their models, they did increase performance in almost all of their models (although not always substantially). They noted that the frequencies of certain concepts or terms in the training set also impacted the resulting model performance and should be taken into consideration.²⁷

As stated previously, we should not be expecting ideal agreement between human coding and Modeler's predicted coding when we are attempting to use written responses to predict responses in an entirely different modality. In fact Beggrow and colleagues have stated "it is not unexpected to find robust (but moderate) correlation magnitudes on tests of the same domain but focusing on different tasks (e.g., oral vs. written vs. selected response)." Indeed, in their own research, they found moderate correlation coefficients when comparing oral interview responses to written responses. They argue that, while their values are not traditionally high, the correlation

between human-scored responses and interviews, as well as computer-scored responses and interviews, were considerably higher than the correlations between the forced-choice assessment and interviews.³¹ While they used different statistical analyses in their study, the same general idea can apply here.

The between drawing model effectively discriminated between student drawing responses that would receive a within or between drawing code based on their written descriptions of hydrogen bonding. These results differ from our previous work with students' text responses, discussed in Chapter X, where we focused solely on students' discussion of IMF location. In Chapter X, we found that many students failed to discuss the location of IMFs in their written responses, making it difficult to determine (based on that information alone) if they understood IMFs to be interactions between molecules or bonds within a single molecule. Modeler, on the other hand, takes into account *all* terms used by students in order to build a predictive model. Our predictive models were better able to predict the drawing code a student would receive based on their written response, essentially highlighting if the student understood hydrogen bonding to occur between molecules rather than within.

It stands to reason that students with a stronger understanding of the forces and interactions taking place would be more likely to include scientific principles in their writing as well as draw IMFs as an interaction between molecules. While our drawing code models did not achieve 100% agreement, they may still be applicable, with further revision, for quickly predicting a students' drawing outcome without actual analysis of their constructed representation. That is, while we certainly encourage instructors to have their students draw and construct representations, applying our model for text analysis could give instructors a quick

approximation of their students' understanding of IMFs without having to pour over hundreds of student drawings.

As for comparing two different introductory general chemistry courses, it appears that the CLUE and traditional students differ in the words they use to describe hydrogen bonding. While both groups use several common terms (i.e. hydrogen, nitrogen, and oxygen) frequently, there are a few key terms that appear to be used predominantly by one group over the other, specifically, CLUE students' allusion to scientific principles with terms such as polarity and interaction, as opposed to traditional students' propensity to use the term carbon. While these differences may seem small, the fact that Modeler can, based on words alone, differentiate between two different GC courses certainly indicates that there must be differences in the way they discuss IMFs and the understanding they derive. CLUE students' tendency to discuss polarity and electronegativity serves as evidence of the effect of the curriculum's increased emphasis on columbic forces, energy, and their impact on molecular interactions. Ideally, we would like students to discuss concepts like molecular shape, electronegativity, and the resulting bond and molecular polarity as contributing factors to the type and strength of IMFs a molecular compound is likely to exhibit. The inclusion of these terms in CLUE students' responses is certainly promising data indicating that the curriculum is succeeding in building these connections. Responses that only mention the elements involved or the strength of IMFs fail to show a solid understanding of the underlying principles that lead to IMFs and are a reflection of the types of information accepted as evidence of understanding the traditional course.

Limitations

One limitation to using discriminant analysis is the need for a large amount of student responses. We were able to create models to predict a student's drawing of hydrogen bonding as occurring within or between molecules, but unfortunately we could not produce successful models for the remaining drawing codes (ambiguous, not present, and student doesn't know) due to the low number of responses. More submissions from students who express these ideas in their drawings would be required to pursue building robust models for these codes.

Additionally, in this study we only explored one IMF (hydrogen bonding) and thus used only one written response and one drawing from each student. By focusing on hydrogen bonding, we were less likely to a thorough discussion of scientific concepts like electronegativity or polarity because many students do not need to use these ideas to predict the IMF present; they can often successfully rely the presence of hydrogen directly bonded to nitrogen, oxygen, or fluorine. Future work would benefit from exploring multiple explanations from students about the same topic to create a more rounded picture of their understanding and improve our models. We do have students' discussions and drawings of dipole-dipole and LDFs that have yet to be explored using text analysis.

It is important to note that, while we did have enough written responses to create predictive models, we did not have enough to create a second data set to test our models. Ideally, we would want to test the reliability of our models on a new group of student responses to determine if the models consistently predicted human scoring. Because we were unable to do so, it is hard to make claims about the models' performance beyond the data set used here. REFERENCES

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CHAPTER IX: CONCLUSIONS, IMPLICATIONS, AND FUTURE WORK

My research has focused on the exploration of students' understanding of the relationship between structure and properties and the role of intermolecular forces. Specifically, I completed four main studies to identify how students connect structure and properties, how they write about and represent intermolecular forces (IMFs), how a reformed curriculum (Chemistry, Life, the Universe, and Everything - CLUE) affects students' understanding of IMFs, and how we can expedite the analysis of written and drawn responses on the Intermolecular Forces Assessment (IMFA).

Conclusions

Main study 1: Students' understanding of structure-property relationships

As discussed in Chapter 4¹, we interviewed students enrolled in both general and organic chemistry to explore how they understood the connection between structure and properties. We found that students possessed a wide range of diverse ideas; in fact, no two students answered our interview questions in the same manner and, as a result, we uncovered several different approaches that were used to discuss properties such as boiling and melting. Many students relied on heuristics, both personal and taught, to explain relative trends in boiling points. These heuristics were often consistently used, although they did not always lead to the correct answer. Others explained these physical processes using a collection of fragmented ideas, akin to diSessa's p-prims², woven together to form an explanation. Typically, these ideas were not consistent since they were often dependent on the prompt. Some students struggled with the terminology used in chemistry courses, like the differences between bonds and interactions, while others found it difficult to construct appropriate representations of phases, drawing lattice structures or breaking apart molecules.

We saw from students' responses that classifying their ideas as "misconceptions" was too simplistic an approach. Many of the explanations voiced by students contained an assortment of ideas, pieced together to answer the question at hand. This was particularly apparent with organic students who included irrelevant concepts such as steric hindrance or the inductive effect to explain boiling and melting processes. Dual process theory can serve as a lens through which we can better understand these responses.³ Several students often altered their answer choice after spending additional time thinking about the question. For instance, when Joy was asked if ethanol or ethane would have the higher boiling point, she originally picked ethane, stating "I wanna say this one has an O, a hydroxyl group on it, so I feel like it would boil quicker than the hydrocarbon." But after further discussion, she changes her response to ethanol:

Joy: Wait, actually I lie. I think this [ethanol] has the higher boiling point. *Interviewer*: Ok so what would you think, that the bonding was there before, so you drew it out and said that now it has hydrogen bonding so...?

Joy: Well I wasn't really thinking about it then. I just looked.

With Joy, it is rather obvious that her initial reaction to ranking boiling points only invoked a System 1 response. It was only after she had taken the time to think through the question that she realized ethanol was capable of hydrogen bonding and thus had the higher boiling point of the two.

Main study 2: Exploring students' understanding of intermolecular forces through writing and drawing

Our work exploring students' understanding of IMFs through written and drawn responses on the IMFA was described in Chapter 6⁴. While we would hope students understand IMFs as interactions that occur *between* small molecules, the majority of students in this study represented IMFs as bonds *within* a single molecule of ethanol. The numbers we have reported are certainly larger than what has been previously discussed in the literature.^{5–7} Previous studies, however, often used multiple-choice assessments to determine where students believed IMFs to be located. I would argue that the act of selecting a correct answer from a set of four possible choices is inherently different than constructing a representation and drawing IMFs, which is more likely to make key structural information apparent.

While students' representations of IMFs clearly depicted their understanding of the interactions as within or between molecules, their written responses were far more ambiguous. Most students did not discuss the location of IMFs, instead citing surfacelevel definitions such as the strength of a given IMF or the elements involved. Few students discussed IMFs as electrostatic interactions, but this is not entirely surprising considering we did not ask for these details in our question prompts. In hindsight, the format of our short answer questions was less likely to invoke a System 2 response from students than questions probing for deeper understanding. For instance, describing hydrogen bonding as the strongest intermolecular force, requiring the presence of hydrogen and nitrogen, oxygen, or fluorine is a completely legitimate response to the

question we asked. A discussion of future work below will outline some ideas to improve the design of the IMFA or create a new, sister assessment.

Perhaps the most important finding from this study was that we would have been unable to determine, from students' writing alone, whether they understood IMFs to be interactions between molecules rather than bonds within a molecule. It was only when we consulted students' drawings that we could make this distinction. By requiring students to draw a representation of IMFs, we were essentially asking them to articulate their ideas and communicate them in a manner that is more likely to reveal spatial information, which is crucial for IMFs. While most students' written responses were ambiguous, some were completely contradictory. In the case of dipole-dipole, several students described the interaction as between molecules but provided a representation as a bond within ethanol. We are not entirely sure as to the cause of this contradiction, but it is clearly evidence of a disconnect in student understanding.

Main study 3: Comparing the effect of a reformed curriculum on students' understanding of intermolecular forces

In Chapter 7, we discussed the effects of the CLUE curriculum on students' understanding of IMFs through analysis of their drawings. We found that the majority of CLUE students from Cohort 1 consistently represented all three IMFs as interactions *between* molecules, unlike the majority of traditional students who represented IMFs as *within* molecules. We attribute this difference to the design of the CLUE curriculum, which emphasizes the interconnectivity of structure, properties, and energy throughout the year. The replication of these results in the data collected from Cohort 2 further supports the positive impact of the CLUE curriculum on student understanding of IMFs.

In addition to collecting IMFA data from Cohort 1 and Cohort 2 at Clemson University, we also administered the IMFA to students at Michigan State University (MSU) to determine if CLUE had the same impact on student understanding when introduced at a new university. While we could not make statistical comparisons between MSU and Clemson students, it does seem that CLUE students at MSU are just as likely as those at Clemson to represent IMFs as interactions between molecules. Traditional students at MSU received fewer within molecules codes for their representations of IMFs than those at Clemson. Instead, we saw an increase in codes such as "ambiguous", "not present", and "student doesn't know". We also noted that students at MSU had more difficulties constructing appropriate structures of ethanol, which made coding their responses more difficult. This is not entirely surprising, however, as these students were never asked on examinations or homework to construct representations of molecules.

Finally, we followed a subset of students from general chemistry through organic chemistry to determine the lasting effects of the CLUE curriculum on students' understanding of IMFs. While our sample sizes were much smaller (it is difficult to follow students longitudinally through organic chemistry), we found that CLUE students still represented IMFs as occurring between molecules after a full year of organic chemistry and traditional students still represented them as within molecules. These results indicate that the effects of the CLUE curriculum are not temporary, rather the ideas that students form during their time with the CLUE course stick with them through subsequent chemistry courses. On the other hand, this also means that a full year of

organic chemistry does little to effect students' understanding of IMFs. Many majors only require students to take two years of chemistry. The ideas about IMFs that traditional students leave general chemistry with are most likely the ideas that they will retain.

Main study 4: Automated text analysis of IMFA responses

In the previous chapter, we outlined the possibility of using automated text analysis to quickly and efficiently analyze students' responses from the IMFA. We explored two different aspects of analysis: 1) using discriminant analysis of students' text responses to predict their location drawing codes and 2) using web diagrams and discriminant analysis to identify differences in CLUE and traditional students' responses. We were able to build moderately successful models to predict the location drawing code (between or within) a student would receive for hydrogen bonding from their written descriptions of hydrogen bonding. It was encouraging to see lexical categories (LC's) like *Electronegativity* and *Polarity* used as strong indicators by our model to predict the presence of the "between" molecules code. It makes sense that a solid understanding of these concepts would be linked to an understanding of IMFs as interactions between molecules. Similarly *Bond* and *Carbon* make sense as strong predictors of the presence of the "within" molecules code; these ideas are often inappropriately associated with hydrogen bonding.

While these models were able to determine the presence or absence of a location code (be it between or within), they were not robust enough use on new sets of data. Our models displayed fairly high percent agreement, but produced only moderate Cohen's

kappa values. This was not entirely surprising, however, considering we were using responses in one modality to attempt to predict the code a student would receive in another modality. We could possibly improve these models by using larger sets of data. By creating robust models, instructors would be able to give the IMFA to their students at several time points and quickly determine how their students are representing IMFs to gauge general understanding.

We were also able to construct web diagrams of CLUE and traditional students' descriptions of hydrogen bonding and identify key differences. For instance, CLUE students made more links to LC's such as *Polarity* and *Interaction* while traditional students possessed more links to the LC *Carbon*. Similarly, we were able to use discriminant analysis to build a model that could effectively differentiate between CLUE and traditional student responses. The fact that our model used LC's such as *Electronegativity* and *Interaction* highlights the effects of the CLUE curriculum on students' understanding of IMFs. The CLUE curriculum explicitly connects intermolecular forces back to shape, polarity, and electronegativity, promoting meaningful learning, and this is reflected in the our discriminant model.^{8,9}

Implications

The positive impact of the CLUE curriculum: Scaffolding structure-property concepts

We believe there are several factors that explain why the CLUE curriculum appears to have such a strong impact on students' understanding of IMFs. As discussed previously, the CLUE curriculum is grounded in theories of how students learn and is intentionally designed to reflect the tenets of meaningful learning. It provides students with a solid foundational knowledge of the core concepts of structure, properties, and energy early in the first semester so that new ideas and topics can then be readily connected back to these foundational concepts. The curriculum emphasizes the interconnectedness of these three core ideas throughout the entire one-year course. Table 9.1 and 9.2 shows the order of topics that are addressed both in the CLUE course as well as the traditional textbooks used by GC courses at Clemson University (CU) and Michigan State University (MSU).^{10–13}

Chemistry, Life, the Universe, and Everything (CLUE) – CU and MSU	General Chemistry: Atoms First – Traditional GC, CU	Chemistry Volume two – Traditional GC, MSU
 1) Atoms Scientific theories Atomic theory and evidence Atomic structure Interactions between atoms and molecules 2) Electrons and Orbitals Light and quantum mechanics Spectroscopy The periodic table 3) Elements, Bonding, and Physical Properties Elements and their interactions Discrete vs. continuous molecules Molecular orbital theory Metals 4) Heterogeneous Compounds 3D and 2D representations Lewis structures and shape Shape, polarity, and interactions Ionic bonding 5) Systems Thinking Kinetic energy and temperature Energy and gases 	 Chemistry: Matter and Measurement Elements and the Periodic Table Units and stoichiometry The Structure and Stability of Atoms Atomic theory and nuclear chemistry Periodicity and the Electronic Structure of Atoms Light and wave-particle duality Quantum mechanics Ionic Bonds and Some Main-Group Chemistry Molecules, ions, and bonds Covalent Bonds and Molecular Structure Electronegativity Lewis structures and shape Molecular orbital theory Mass Relationships in Chemical Reactions Types of reactions Thermochemistry: Chemical Energy Energy and enthalpy Entropy and free energy Gases: Their Properties and Behavior Gas laws 	 1) Chemistry Measurement Atoms and molecules 2) Stoichiometry 3) Reactions in Solution Oxidation Reduction Reactions in aqueous solutions 4) Energy First law of thermodynamics Changes of state Enthalpies of reactions 5) Atomic Structure Periodic properties 6) Bonding and Molecular Structure VSEPR Molecular orbital theory 7) States of Matter Gases and gas laws Kinetic molecular theory Intermolecular forces 8) Thermodynamics, Phase Diagrams and Solutions Changes of state
- Phase changes	10) Liquids, Solids, and Phase Changes	

Table 9.1: Table of contents for the material covered in the first semester of each general chemistry course

Chemistry, Life, the Universe, and	General Chemistry: Atoms First –	Chemistry Volume two – Traditional
Everything (CLUE) – CU and MSU	Traditional GC, CU	GC, MSU
 6) Solutions Solubility and Gibbs energy Polarity and solutions Temperature and solubility 7) A Field Guide to Chemical Reactions Collisions and reactions Collisions and reactions Acid-base Nucleophiles and Electrophiles Oxidation Reduction 8) How Far? How Fast? Factors that control reactions Reaction rate Kinetics and activation energy Equilibrium 9) Reaction Systems Buffered reactions Coupled non-equilibrium reaction systems 	 11) Solutions and Their Properties Energy changes Colligative properties 12) Chemical Kinetics Reaction rates and rate laws 13) Chemical Equilibrium Factors that affect equilibrium Equilibrium and kinetics 14) Aqueous Equilibria: Acids and Bases pH and acid-base theories Equilibrium and strength 15) Applications of Aqueous Equilibria Buffers and titrations Factors that affect solubility 16) Thermodynamics: Entropy, Free Energy, and Equilibrium 17) Electrochemistry 18) Hydrogen, Oxygen, and Water 19) The Main-Group Elements 20) Transition Elements and Coordination Chemistry 21) Metals and Solid-State Materials 22) Organic Chemistry 	 Chemical Kinetics Mechanisms Rates of reactions Aqueous Equilibria Acid and Bases Solubility equilibria Thermodynamics First and second law of thermodynamics Electrochemistry Chemistry of the Main Group Elements Chemistry of the Transition Elements Coordination compounds Ligand field theory and MO theory Nuclear Chemistry Fission and Fusion Organic Chemistry and Biochemistry

Table 9.2: Table of contents for the material covered in the second semester of each general chemistry course

The CLUE curriculum, as shown in Table 9.1, begins with a discussion of atomic theory, energy, and how atoms interact. This initial conversation introduces students to the idea that atomic interactions are governed by differences in charge, which provides the foundation for future discussions of how and why molecules interact. After examining current atomic theory using basic quantum mechanics, the CLUE curriculum begins to introduce the relationship between structure and properties for molecular compounds. Students are encouraged to think about properties that they know of for diamond and graphite, two substances that are composed entirely of carbon atoms, before entering a discussion of how these properties relate back to differences in structure on the molecular level. Here, the connection between structure and properties is made explicit for students and is discussed in terms of familiar macroscopic phenomena.

Figure 9.1 shows the progression of topics discussed in the CLUE curriculum over the course of Chapters 3, 4, and 5 to link molecular structure and properties. Each of the topics introduced in Figure 9.1 is clearly connected to the previous concept(s) that came before it. By discussing the relationship between these topics, we can help students better understand the complex connection between structure and properties. The CLUE curriculum's discussion of intermolecular forces encourages students to recall previous conversations on electrostatic interactions between atoms as well as the topics of electronegativity and polarity. The topic of IMFs is ultimately connected to larger concepts such as what happens at the molecular level during a phase change and solute-solvent interactions when discussing solubility.



Figure 9.1: The progression of topics discussed in CLUE to connect molecular structure and properties. Reprinted with permission from Cooper, M. M.; Underwood, S. M.; Hilley, C. Z.; Klymkowsky, M. W. *J. Chem. Educ.* **2012**, *89*, 1351–1357.¹⁴ Copyright 2015 American Chemical Society.

Unlike the CLUE curriculum, the traditional textbooks used by Clemson and MSU fail to meet the tenets of meaningful learning^{8,9}; IMFs are typically separated, both from the foundational material needed to understand them (Lewis structures, geometry and electronegativity), and from the physical and chemical properties that they help explain (solubility, phase changes). For instance, the traditional GC text used at Clemson University, *General Chemistry: Atoms First*, discusses Lewis structures, geometry, and polarity in Chapter 5, seen in Table 9.1, but does not begin to discuss IMFs or properties until Chapter 10.¹¹ Both curricula at Clemson and MSU include an extensive discussion of gas laws and kinetic molecular theory after introducing molecular structure and polarity but before a discussion of IMFs and properties of molecular substances. The CLUE curriculum explicitly connects these ideas and emphasizes the three core concepts of structure, properties, and energy throughout the course.

This emphasis is reflected in our IMFA results and it is clear that making these connections explicit positively impacts students' understanding.

The positive impact of the CLUE curriculum: Engaging in scientific practices

In addition to focusing on core chemistry concepts and using a scaffolded approach to introduce and teach these concepts, the CLUE curriculum engages students in scientific practices and encourages group work and discussion. Students are asked to build scientific explanations and arguments as well as construct representations in in-class assignments, homework, and even on exams. For instance, when learning how to draw Lewis structures, CLUE students are provided molecular modeling kits in class and encouraged to work together in groups to build three-dimensional representations of assigned molecules and translate those representations to two-dimensional Lewis structures. Students are also asked to practice constructing appropriate Lewis structures for homework through *beSocratic* and later on asked to use these structures to represent molecular interactions in a variety of ways (i.e. solute-solvent interactions, acid-base reactions, and IMFs). CLUE exams consist of a combination of multiple-choice and constructed-response assessment items. These constructed-response items often require students to write explanations, draw graphs, and depict representations of various chemical and physical phenomena.

While the traditional course at Clemson could be considered reformed in that students used clickers and completed group assignments, neither traditional course at Clemson or MSU emphasized the need to construct representations, scientific explanations, or arguments. In fact, students at MSU are never given the opportunity in lecture or for homework to draw Lewis structures. Both universities use a standard online

homework management system (like Mastering Chemistry¹⁵) that does not require students to construct representations. Additionally, traditional exams at both universities consist entirely of multiple-choice questions. As we have seen from our work with the IMFA, asking students to construct representations can reveal student understanding that would be otherwise unapparent in written responses or in answers to multiple-choice questions. Constructivism tells us that knowledge is constructed in the mind of the learner.¹⁶ How can we expect students to effectively develop and communicate ideas if we have never asked them to express their understanding and reconstruct it? As we have seen with the CLUE curriculum, giving students the opportunity to engage in these scientific practices can enhance their understanding of core ideas and provide them with a more realistic understanding of how science happens.¹⁷

We believe that the CLUE curriculum's focus on the three core chemistry concepts (structure, properties, and energy), its scaffolded approach to teaching these concepts, and its emphasis on scientific practices can help explain why CLUE appears to have such a positive impact on students' understanding of IMFs. The CLUE curriculum explicitly ties the topic of IMFs to each core concept and students are asked to develop and demonstrate understanding of IMFs through the use of scientific explanations and constructed representations.

Implications for assessment

Our structure-property interviews have shown that students can effectively answer boiling point ranking tasks with little understanding of the underlying scientific concepts and ideas. Often students used heuristics to explain these trends. That is not to say that

heuristics are necessarily bad; experts use them, too. And it can certainly be argued that developing schema to expedite knowledge retrieval is necessary to make it through any chemistry course. These shortcuts are essential to reduce cognitive load and prevent overwhelming working memory.^{18,19} However, if students' heuristics are not based on a solid, foundational understanding of the relevant chemistry topics, then heuristics only succeed in masking an underlying lack of understanding. Assessment items that can be easily answered with heuristics are doing a disservice to students. They often fail to highlight deep understanding and instead reward memorization and rote learning.

Our reliance on multiple-choice assessments has contributed to the problem. Multiple-choice questions are useful and sometimes necessary (especially for large class sizes) but there are additional, and often times better, ways uncover to student understanding. We have also shown in our work with the IMFA that question format is important; if the intent of a question is to uncover student understanding related to spatial information, then questions requiring students to draw may be more beneficial. We should be encouraging our students to build scientific explanations, use models, and construct representations. These practices should be reflected both in summative assessments, like exams, as well as formative assessments like homework and in-class assignments, as discussed earlier.

With modern improvements in text analysis, it is already possible to code large data sets of text responses for the presence or absence of themes and ideas.^{20,21} Hopefully, these advances will encourage instructors to expand beyond multiple-choice tests as this technology becomes more available. In an effort to make text analysis more accessible, the Automated Analysis of Constructed Response group (AACR) at MSU has put their

questions and models online for instructors who would like to use them in their own courses and look for the presence of alternative biology ideas. Examples include questions pertaining to ecosystems, evolution, cellular respiration, and strong versus weak acids and bases²² They are currently working to expand their studies to include questions in chemistry and mathematics fields. In the same vein, it may be possible, with more work, to use students' writing to predict aspects of their constructed representations (like our work with the IMFA), which could allow instructors to give a variety of assessments while still quickly and consistently coding/scoring responses for relevant information and ideas.

Future work

We have two future projects planned to extend the work described here. The first is to administer the IMFA at several universities of varying types and sizes across the country. While we have data from Clemson University and Michigan State University, as well as a small collection for a residential college within MSU, we would like to be able to determine if our findings from the IMFA are reflected in other educational settings. It may be that traditional students at Clemson and MSU experience more difficulties representing and describing IMFs than other universities, but we do not believe this is the case. By collecting similar responses from other institutions, we can highlight the extent of students' confusion of IMFs with covalent bonds.

Our second project would require either revision of the IMFA or the creation of a new, sister assessment(s). We now understand that some of the short answer questions included in the IMFA do not appear to uncover deep student understanding of the

scientific concepts behind IMFs and why they occur. Rather, students' written responses to the IMFA were more surface-level and seemed to invoke a System 1 response.³ We also never asked students in our assessment to use their understanding of IMFs to predict and explain various properties like boiling and melting points. A second (or even third) assessment would most likely incorporate the drawings slides from the IMFA and focus on these two additional aspects of IMFs.

Questions probing polarity and electronegativity could help identify if students understand their role in determining the type and strength of IMFs that a molecule would exhibit. Possible items could be providing students with a clear depiction of hydrogen bonding using methanol and water and asking them "Why does this interaction occur between the oxygen in water and the hydrogen covalently bonded to oxygen in methanol? What do you think is causing this interaction?" We could also inform them that the oxygen in water does not interact with the hydrogens covalently bonded to carbon and ask them to explain why that is.

Perhaps more difficult will be designing questions that effectively require students to connect their knowledge of IMFs to physical properties. We have made past attempts to uncover these ideas using assessment items and have not had much success. It may be that our questions were not directed enough that the information we were hoping to assess. For instance, we have given students the structure of an amino acid and ask them to predict and explain any properties it might have. Our intention was to see what properties students would identify and if they would relate them to the structure. Instead, however, responses varied widely in the type of properties predicted and few were ever explained or explicitly connected to the Lewis structure. Like some of our IMFA short

answer questions, the amino acid question may have been too broad. Questions asking students to represent interactions between molecules and explain how these interactions affect the boiling point could be one possible direction. REFERENCES

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Appendix B: Full structure-property interview protocol

Here we provide the full interview protocol:

Part 1: Structure and Properties of water, ammonia, and ethane

- 1. If you had an unknown compound in lab, what kinds of tests might you run to figure out what it is?
- 2. What kind of properties does water have?
- 3. Does the molecular-level structure affect these properties (mentioned in #2)?
- 4. What types of representations are used to show the molecular-level structure?
- 5. Which do you use?
- 6. Can you draw the structure of water and explain how you would use it to determine the properties you have talked about?
- 7. What is the shape of the water molecule? Does this affect the properties? *Repeat questions #2-7 for ammonia and ethane

Part 2: Comparing properties

- 1. Compare CH₃CH₂OH and CH₃CH₃
 - a. Do they have different boiling points? If so, which is higher?
 - b. Why
- 2. Compare CH₃CH₂OH and CH₃OH
 - a. Do they have different boiling points? If so, which is higher?
 - b. Why
- 3. Compare CH₃CH₂OH and CH₃OCH₃
 - a. Do they have different boiling points? If so, which is higher?
 - b. Why

Part 3: Deducing properties of an unfamiliar structure

*The interviewer provides the interviewee with the Lewis structure of acetamide:

- 1. What properties do you think this substance would possess based on the structure?
- 2. Why?

Appendix C: Additional examples of structure-property interview themes

Here we provide additional examples of each overarching theme

Inappropriate Models of Phases or Phase Change:

Like Joe and Jill difficulties with depicting ethane as a solid, Joy (OC2) struggled to visualize ethane in liquid form. Her first instinct was to bond them together into a structure that resembled butane, drawing a long connecting line between two ethane molecules. After further thought, however, she stated that she could not depict the interaction on paper:

Interviewer: So two ethane molecules would interact to form butane? *Joy*: No they're still probably going to be ethane like, like in liquid form you know you just add it to each other but on this paper I can't see the interaction.

Jane (OC2) also struggled with her understanding of phase and phase changes. Upon first impression, it appeared that Jane had a coherent understanding of the phase change from liquid to gas:

Jane: Ok, so if it's boiling, this hydrogen bond should break. And oxygen, oxygen uhh I mean water molecule become, becomes gas phase.

Interviewer: Ok. So if that's going from umm liquid to gas for boiling, then what happens when water melts? So from solid to liquid?

Jane: Mmm I don't know...umm like probably in solid phase they are very, very, very, very close to each other. And umm when they transfer to liquid, the distance would be a little far, but it's not that far. So the hydrogen bond, the molecular, the intermolecular uhh force should still exist.

It only became apparent after further questioning, however, that for Jane intermolecular forces were **only** present in the liquid phase.

Jane: I think the intermolecular force is talking about, is talking only in liquid phase.

Interviewer: How is ice structured then? Like what holds it together?

Jane: Probably the, the, I mean the, since the temperature is very low, umm the activity of each molecule is, is very low. So they are umm, they're very stable at where they are.

Her assertion that in solids there are no intermolecular forces, seemed to imply that at lower temperatures the atoms just "lie down" next to each other, but that there are no forces keeping them there (except perhaps for gravity). This could be another manifestation of a p-prim invoking a macroscopic phenomenon at the molecular level.

Representational difficulties:

Lucy's difficulties with the polarity of dimethyl ether were not unique. Robin (OC1) presented similar issues with translating between 2-dimensional structures on paper and their actual 3-dimensional shape, particularly with the interaction of water molecules.

And so um if you have multiple water molecules they're going to line up like negative positive, negative positive, negative positive like that...and so that's going to be um a pretty rigid structure especially in ice um it's going to keep it together and also um because they're interacting with each other so closely like the negative is right up there with the positive.

Rather than the 3-D structure of ice that would result from the tetrahedral shape of the electron pairs in water, she envisages a linear chain of water molecules in the solid state (ice).

Language and Terminology issues:

In the paper, we provided examples of students' difficulties with the terms intermolecular, intermolecular, and hydrogen bonding. Marshall (OC2) also had terminology issues with the term hydrogen bonding. He, like Ted, believed that hydrogen bonding was a bond within the molecule, which created problems when he started to talk about its strength in comparison to ionic and covalent bonding:

Marshall: It's (hydrogen bonding) a bond between a hydrogen atom and then either an oxygen atom, a nitrogen atom, or a fluorine atom.
Interviewer: Is it a real one or is it just like, like ok so you have your different strength of bonds right?
Marshall: Yeah.
Interviewer: So you have ionic you were talking about and covalent.
Marshall: Yeah.
Interviewer: Umm so where would like a hydrogen bond fit?
Marshall: Umm I would say in between ionic and covalent.

After further questioning it became apparent that he had the definitions of ionic and covalent bonding confused. When asked to explain an ionic bond, Marshall stated, "It's a bond between two nonmetals". Conversely, he described a covalent bond as being "between a metal and a nonmetal". The concept of bonding alone is nontrivial, but adding in the idea of intermolecular forces can exacerbate misunderstandings if not properly incorporated.

Other students, however, were unsure of the difference between "reaction" and "interaction" of molecules, sometimes providing a reaction when asked if the molecules interacted. In this example, Joy (OC2) was asked if two molecules of ethanol would interact. She responded, "Mmm I feel like I would, I feel like I would lose water if I tried to interact these two. I feel like I would end up with an ether". Indeed, two ethanol molecules can react to form an ether, but the intent of the interviewer was that she would discuss intermolecular forces between the two molecules using terminology commonly found in chemistry courses. Subsequently, Joy elaborated on the differences between reacting and interacting: "Hmm reacting and interacting. When I think react I just I think of like a chemical equation...Interact I don't know. I just feel, think of the pictures in the book. Or like water or something being lost".

Use of Heuristics in Student Reasoning:

Heuristics – Instructionally derived: Instructionally derived heuristics have been devised to provide students with tools that lower the cognitive load of the task and allow them to make predictions. One example consists of the "octet rule", which is a heuristic designed to aid students in constructing appropriate Lewis structures for simple compounds; however, what students often do not understand is that it only works for predicting four (C, N, O, F) out of the current 112 elements. Daisy (OC2) is one example of a student who invoked the octet rule for ethane to argue that octets are the reason for stability resulting in lack of reactivity: "Umm well it's carbon. You said ethane? So it's a pretty happy little molecule. All the octets, the oc- well all

the octet of the carbons are filled so it's pretty stable".

"Like dissolves like" is another example of a instructionally derived heuristic that can lead to didaskalogenic problems if it becomes the only reasoning to explain solubility. This heuristic only serves as a rule and fails to provide the explanation as to why the solute is soluble in a given solvent. While Erin (OC2) uses the "like dissolves like" heuristic to discuss the polarity differences for ethane in water to predict its insolubility, Noah (GC2) uses it more broadly to explain the interaction of organic and inorganic compounds. "Umm...organic compounds are usually water-soluble anyway, aren't they? No wait, why would they be water-soluble...Because what is it, like water is inorganic and these are organic so no". Noah proceeds to correct himself and discuss instead the attraction between molecules. This is an example of how easy it is for students to spontaneously use heuristics without considering their underlying conceptual basis. If care is not taken to explain the origins of these heuristics, students can even misapply them to inappropriate situations.

Heuristics – "*More means more*": Marshall (OC1), similar to Robin (OC1) in the paper, uses this reasoning when comparing ethanol and methanol. He argues that ethanol is a heavier molecule, which results in a higher boiling point: "I am just trying to think. Like I know that this like one [ethanol] is, that one's a bigger molecule...I guess that would give it a higher boiling point...If it's a bigger molecule it would need more energy to like move around so...uh yeah I guess it would be in order to move from a liquid phase to a gaseous phase it would need more energy".

Appendix D: Interview students' explanations and representations of IMFs

Table A.1: Written descriptions and drawn representations of IMFs from our interviews

Student pseudo- nym	IMFs initially identified	IMF Description	IMF Representation
	Hydrogen bonding	"Since it's more electronegative, you get an interaction between those two (oxygen and hydrogen)."	
Jamie	Dipole- dipole	"Basically it has positive and negative ends on the atomsyou'd have a weak bond sitting right here (between the two molecules). "	$\frac{1}{4} + \frac{5}{4} + \frac{5}{4} + \frac{5}{4} + \frac{1}{4} + \frac{1}$
	Van der Waals	"Electrons in the orbital they move around so if they're moving more in this bond then it's going to be more positive herelike if you have more electronegative molecule, the electrons will side more on that side."	
	Hydrogen bonding	"That's just, it's umm H, I mean it's C, N, O, and F I'm pretty sure. All of experience hydrogen bonding. And I know they're pretty weak; they're pretty easy to break."	Initially within molecules:
Margery	Dipole- dipole	"You can have something that's going to have a partially negative and a partially positive charge, butthe electron sharing will be a lot more equal."	ON COS
	Van der Waals	"Basically all, everything experiences Van der Waals forces. It's because I think they're like momentary dipoles, like everything that's bonded at one point or another experiences a partial positive/partial negative charge."	6t 8- H-O

Table A.1 (cont'd)

Robert	Hydrogen bonding	"I know oxygen and nitrogen are in hydrogen bonding, so I guess any sort of electronegative atom with hydrogen attached to it."	Within and between molecules: $H = \frac{0}{10} + \frac{1}{10} + \frac{1}{10$
1.000	Dipole moment	"Any bond has, between two atoms is going to have some sort of dipole moment."	р ^о — Н
	Van der Waals	Could not describe	N/A
Caitlyn	None	Did not remember any IMFs, even after prompting	N/A
	Dipole- dipole	Could not describe	N/A
John	Van der Waals	"It's just the attraction between electrons holding it together. It's a pretty weak force I guess."	60
	*Hydrogen bonding after prompting	"Umm it's just like an electronegative molecule is attracted to the hydrogen, I mean the hydrogens can like donate a proton."	$(1)^{-1}$ $(\#)^{-1}$



Appendix E: Copy of the initial Intermolecular Forces Assessment with a student's responses

Figure A.1: A copy of the initial IMFA given on paper with one students' response

Figure A.1 (cont'd)

If you had two molecules of this Molecular Level Picture (3-4 molecules) Structure Intermolecular Forces structure, would they interact? Explain. Hydhogen bunds are kind of Weak Nb. This molecule is saturated. have ho So they alen't very stray. Yes. Nish' ND I have no earthly idia. full with CW. Valera election s.

-1

Appendix F: Examples of students' representations of dipole-dipole interactions and London dispersion forces



Figure A.2: Student representations of dipole-dipole that received (a) between code, (b) within code, (c) ambiguous code, (d) not present code, and (e) student DK code



Figure A.3: Student representations of LDFs that received (a) between code, (b) within code, (c) ambiguous code, (d) not present code, (e) student DK code, and (f) always present code

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Appendix I: Demographic and pre-instruction assessment data for Cohorts 1 and 2

Here we provide demographic and pre-instruction assessment information for Cohorts 1 and 2. Data shown below includes sex, common majors, SAT composite scores, Metacognitive Activities Inventory (MCAI) scores¹, Students' Understanding of Models in Science (SUMS) scores², and Implicit Information from Lewis Structures Instrument (IILSI) scores³. These measures were all collected early in the first semester of the students' general chemistry course (GC1).

The MCAI, which contains 27 items using a 5-point Likert scale, was designed to assess how students' think about their own problem-solving skills in the context of chemistry. The SUMS instrument consists of 27 items, each with a 5-point Likert-type scale ranging from "strongly disagree" (1) to "strongly agree" (5). The instrument was designed to examine students' understanding of models and use of models through five different scales: Models as multiple representations (MR), Models as exact replicas (ER), Models as explanatory tools (ET), Uses of scientific models (USM), and The changing nature of models (CNM). The IILSI is a one-question instrument, requiring students to select all items that apply out of 17 possible items. The IILSI is designed to explore what properties students' believe they can determine from the structure of a molecule.

Demographics	Cohort 1 (N=94)	Cohort 2 (N=160)
Sex	67% Female, 33% Male	73% Female, 27% Male
Maiona	30% Biological Sciences,	32% Biological Sciences,
wiajors	18% General Engineering	16% Animal and Veterinary Sciences

Table A.2: Sex and most common majors for Cohort 1 and Cohort 2

Table A.3: Pre-Instruction scores on SAT composite, MCAI, and SUMS for Cohorts 1 and 2

	A	
Pre-Instruction Assessments	Cohort 1 (N=94) Mean	Cohort 2 (N=160) Mean
SAT Composite (out of 1600)	1248	1227
MCAI (out of 100)	78.5	76.6
ET – SUMS	4.32	N/A
ER – SUMS	4.32	N/A
USM – SUMS	3.78	N/A
CNM – SUMS	3.43	N/A
MR – SUMS	4.32	N/A

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Pre-Instruction IILSI	Cohort 1 (N=94) Mean	Cohort 2 (N=160) Mean
No information	1%	2%
Element(s) present	80%	79%
Number of valence electrons	86%	83%
Number of bonds between	800/	7104
particular atoms	8970	/ 1 70
Type of bond(s)	93%	79%
Formal charges	65%	22%
Bond angle	49%	36%
Geometry/shape	58%	53%
Potential for resonance	48%	8%
Hybridization	25%	17%
Polarity	58%	51%
Intermolecular forces	30%	14%
Acidity/basicity	13%	18%
Reactivity	24%	28%
Relative boiling points	10%	8%
Relative melting points	8%	6%
Physical properties	17%	22%

Table A.4: Pre-Instruction performance on all 17 IILSI items for Cohorts 1 and 2

Appendix J: A comparison of all drawing and text code frequencies for Cohorts 1 and 2

As stated within the chapter, our coding scheme for students' drawings of IMFs included several major code categories: within, between, ambiguous, within and between, student DK and not present. An additional category of "always present" was possible for students' representations of LDFs. For the sake of simplicity, we provided figures with only "within" and "between" code frequencies. Here we provide the code frequencies of all possible drawing codes as shown in Figure 2 for Cohorts 1 and 2.



Figure A.4: Comparison of all drawing code frequencies for Cohort 1 and 2

Appendix K: Demographic and pre-instruction assessment data for CLUE and traditional students in all three cohorts as well as statistical comparisons for Cohorts 1 and 2

Here we provide basic demographic information, like sex and common majors, as well as pre-instruction assessment scores for all three cohorts included in our study. For Cohort 1, pre-instruction measures included SAT composite scores, Metacognitive Activities Inventory (MCAI) scores¹, Students' Understanding of Models in Science (SUMS) scores², and Implicit Information from Lewis Structures Instrument (IILSI) scores³. For Cohort 2, we provide SAT composite scores, MCAI scores, and IILSI scores. We do not have pre-instruction assessment data, aside from ACT composite scores, from Cohort 3 at Michigan State University (MSU) and therefore do not include chi-square analysis for significant differences between the CLUE and traditional group. All pre-instruction assessments were administered for each cohort early in their first fall semester for the purpose of collecting baseline data.

The MCAI is designed to explore what students think about their problem-solving skills in their chemistry courses and consists of 27 items on a 5-point Likert scale. The SUMS instrument was designed to assess students' understanding of models via 27 items, also using a 5-point Likert scale. These items on the SUMS cover five different ideas: models as multiple representations (MR), models as exact replicas (ER), models as explanatory tools (ET), uses of scientific models (USM), and the changing nature of models (CNM). Lastly, the IILSI was designed to probe students' understanding of the connection between structure and properties by exploring the types of information students' believe they can determine from a molecular structure. The IILSI is a single question assessment with 17 possible item choices, requiring students to select all that may apply.

For both Cohorts 1 and 2, we used pre-instruction assessments to determine if the CLUE and traditional groups were similar within each cohort using a chi-square analysis. We have included group means as well as p-values when applicable. Any p-values showing a significant difference have been bolded. It should be noted that the IILSI for Cohort 1 students was administered after they received instruction on the topic of Lewis structures, which is evident by the student responses. These students had not, however, been instructed on the true purpose for these structures (i.e. predicting chemical and physical properties). When considering the items that both groups had not been instructed on for Cohort 1, we believe that in fact the students within this cohort are equivalent for this measure.

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Cohort 1: Clemson University, Fall 2011 – Spring 2013

Demographics	Traditional	CLUE	p-value
Sex	67% Female, 33% Male	59% Female, 41% Male	0.310
Maiora	30% Biological Sciences,	47% Biological Sciences,	N/A
wiajors	18% General Engineering	10% General Engineering	

Table A.5: Sex and most common majors for Cohort 1 traditional and CLUE groups

Table A.6: Pre-instruction scores on SAT composite, MCAI, and SUMS for Cohort 1 traditional and CLUE groups

Pre-Instruction Assessments	Traditional Mean	CLUE Mean	p-value
SAT Composite (out of 1600)	1248	1260	0.236
MCAI (out of 100)	78.5	78.4	0.806
ET – SUMS	4.32	4.41	0.198
ER – SUMS	4.32	4.41	0.198
USM – SUMS	3.78	3.71	0.454
CNM – SUMS	3.43	3.56	0.371
MR – SUMS	4.32	4.43	0.122

Table A.7: Pre-Instruction performance on all 17 IILSI items for Cohort 1 traditional and CLUE groups

Pre-Instruction IILSI	Traditional Mean	CLUE Mean	p-value
No information	1%	0%	1.000
Element(s) present	80%	85%	0.526
Number of valence electrons	86%	63%	0.003
Number of bonds between particular atoms	89%	78%	0.160
Type of bond(s)	93%	67%	<.001
Formal charges	65%	14%	<.001
Bond angle	49%	44%	0.669
Geometry/shape	58%	49%	0.356
Potential for resonance	48%	9%	<.001
Hybridization	25%	21%	0.725
Polarity	58%	71%	0.128
Intermolecular forces	30%	27%	0.894
Acidity/basicity	13%	13%	1.000
Reactivity	24%	22%	1.000
Relative boiling points	10%	4%	0.337
Relative melting points	8%	4%	0.505
Physical properties	17%	20%	0.797

Cohort 2: Clemson University, Fall 2012 – Spring 2013

Demographics	Traditional	CLUE	p-value
Sex	73% Female, 27% Male	64% Female, 36% Male	0.174
Majors	32 % Biological Sciences, 16% Animal and Veterinary Sciences	74% Biological Sciences, 13% Microbiology	N/A

Table A.8: Sex and most common majors for Cohort 2 traditional and CLUE groups

Table A.9: Pre-instruction scores on SAT composite and MCAI scores for Cohort 2 traditional and CLUE groups

Pre-Instruction Assessments	Traditional Mean	CLUE Mean	p-value
SAT Composite (out of 1600)	1227	1243	0.264
MCAI (out of 100)	76.6	76.2	0.567

Table A.10: Pre-instruction performance on all 17 IILSI items for Cohort 2 traditional and CLUE groups

Pre-Instruction IILSI	Traditional Mean	CLUE Mean	p-value
No information	2%	1%	0.851
Element(s) present	79%	78%	1.000
Number of valence electrons	83%	76%	0.295
Number of bonds between particular atoms	71%	64%	0.279
Type of bond(s)	79%	73%	0.383
Formal charges	22%	22%	1.000
Bond angle	36%	27%	0.182
Geometry/shape	53%	42%	0.118
Potential for resonance	8%	4%	0.106
Hybridization	17%	17%	1.000
Polarity	51%	47%	0.656
Intermolecular forces	14%	22%	0.146
Acidity/basicity	18%	28%	0.436
Reactivity	28%	23%	0.473
Relative boiling points	8%	10%	0.760
Relative melting points	6%	9%	0.493
Physical properties	22%	20%	0.815

Cohort 3: Michigan State University, Fall 2013 – Spring 2014

Table A.11: Sex, most common majors, and ACT composite scores for Cohort 3 traditional and CLUE groups

Demographics	Traditional	CLUE	
Sex	49% Female, 51% Male	55% Female, 45% Male	
Majora	17% Human Biology,	27% Human Biology,	
Wajors	12% Kinesiology	24% Pre-medical	
ACT Composite (out of 35)	26	26	

Appendix L: Chi-square analyses of all drawing code frequencies for CLUE and traditional students in Cohorts 1 and 2

In Table A.12, we have included means, p-values, and effect sizes when appropriate for all drawing codes used for students' responses. Significant p-values have been bolded.

Cohort	IMF	Code	Traditional	CLUE	p-value	4
			percentage	percentage		Ψ
Cohort 1	Hydrogen bonding	Within	72.3	10.3	<.001	0.62
		Between	14.9	82.8	<.001	0.67
		Not Present	4.3	0.0	0.15	
		Ambiguous	3.2	4.6	0.92	
		Within and Between	5.3	2.3	0.51	
	Dipole- dipole	Within	60.6	13.8	<.001	0.47
		Between	10.6	63.2	<.001	0.54
		Not Present	14.9	9.2	0.35	
		Ambiguous	12.8	12.6	1.0	
		Within and Between	1.1	1.2	1.0	
	LDFs	Within	55.3	14.9	<.001	0.41
		Between	11.7	62.1	<.001	0.51
		Not Present	6.4	1.2	0.15	
		Ambiguous	12.8	14.9	0.84	
		Within and Between	0	2.3	0.44	
		Always Present	11.7	4.6	0.14	
		Student DK	2.1	0.0	0.51	
Cohort 2	Hydrogen bonding	Within	56.2	10.2	<.001	0.46
		Between	31.3	83.8	<.001	0.51
		Not Present	1.9	0.0	0.37	
		Ambiguous	7.5	3.4	0.24	
		Within and Between	3.1	2.6	1.0	
	Dipole- dipole	Within	58.1	16.2	<.001	0.41
		Between	15.6	71.8	<.001	0.56
		Not Present	13.8	6.0	0.06	
		Ambiguous	3.7	6.0	0.56	
		Within and Between	1.9	0.0	0.37	
		Student DK	6.9	0.0	0.006	0.16
	LDFs	Within	55.6	12.8	<.001	0.43
		Between	20.0	68.4	<.001	0.48
		Not Present	9.4	4.3	0.17	
		Ambiguous	4.4	9.4	0.15	
		Within and Between	5.0	3.4	0.73	
		Always Present	5.0	0.9	0.11	
		Student DK	0.6	0.9	1.0	

Table A.12: Chi-square statistical analysis results for comparing all drawing code frequencies for CLUE and Traditional students at the end of GC2 in Cohort 1 and Cohort 2

Appendix M: Consistency of students' drawing codes across all three IMFs

While comparisons can provide a snapshot of the differences for a given IMF, we also explored the consistency of students' responses in our paper using Sankey diagrams. Sankey diagrams provide a visual aid that allows the reader to quickly see where most students travel between codes. In Table A.13, we have provided the specific percentages of students who consistently received a particular code for all three of their IMFs representations. These values are only included for students in Cohort 1 since Sankey diagrams were generated for that particular cohort.

Consistency of responses	Traditional (N=94)	CLUE (N=87)	
Within	38%	6%	
Between	1%	46%	
Ambiguous	2%	0%	
Within and Between	0%	1%	
Inconsistent	59%	47%	

Table A.13: Consistency of students receiving a particular drawing code across all three IMFs

Appendix N: Expansion of the "all other codes" category

In our chapter, we compared the traditional students among all three cohorts. While we could not make any statistical comparisons due to a lack of pre-instruction assessments for Cohort 3, we were able to see some general differences between the universities. In Figure A.5, shown below, we expand the "all other codes" category to show the percentages of "ambiguous", "not present", and "student DK" codes.



Figure A.5: Comparison of "other" code category frequencies for all three traditional student cohorts

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