CHARACTERIZING STUDENT THINKING ABOUT SOLUTIONS AND THE SOLVATION PROCESS: THE SEARCH FOR MECHANISTIC UNDERSTANDING

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ABSTRACT

CHARACTERIZING STUDENT THINKING ABOUT SOLUTIONS AND THE SOLVATION PROCESS: THE SEARCH FOR MECHANISTIC UNDERSTANDING

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Chemistry is all about how atoms and molecules interact with themselves and each other resulting in properties and phenomena that can be detected and observed at the macroscopic scale. It follows quite closely then, that an important goal of chemistry education is to help students understand how macroscopic phenomena are governed by interactions and energy changes that accompany changes in interactions at the molecular level. While the literature is filled with examples of ways student incorrectly understand energy across a wide range of topics in chemistry, there is a growing trend to characterize students understanding along a continuum rather than catalog incorrect ideas. This research seeks to characterize how students in a reformed general chemistry curriculum, Chemistry, Life, the Universe and Everything (CLUE), understand solutions and the solvation process in the context of the dissolution of an ionic salt to form an aqueous solution.

Preliminary research uncovered representative ways students successfully and unsuccessfully described an observable temperature change that accompanied the solvation process in a series of student interviews. These findings, as well as reasoning strategies that were observed to help students make connections between atomic-molecular level interactions and energy and macroscopic level temperature changes, were used to design a formative assessment activity targeting this phenomenon. Specific assessment tasks in which students constructed representations and explanations of the

temperature change that accompanied solvation were then operationalized as research tools and administered as formative and summative assessments.

Subsequent analysis of student responses resulted in development of robust coding schemes that were used to characterize how students used mechanistic components in their representations and explanations. In spite of extensive literature describing student difficulties representing solutions, the vast majority of students in the CLUE curriculum were observed to be able to represent the fully dissolved solution as being composed of separated ions each individually interacting with solvent molecules. Further revision of the explanation prompt, leveraging principles influenced by the scaffolding and evidence centered design literature, resulted in a medium to large increase in sophistication of students' use of interactions from representation to explanation tasks; these results were replicated in multiple student populations.

Finally, implications of this work relevant to enacting curricular support for students to use atomic-molecular scale interactions in a mechanistic way are presented, including the importance of designing assessments capable of eliciting evidence of student understanding.

To Carman and Pearl.
Looks like we've made it after all.

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lives, but I will. Knowing you would be there when I got home made everything better. I hope you realize in the future that you really can do what you set your mind to, even if it takes more attempts and time than you think possible, if you really want to.

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CHAPTER 1 — INTRODUCTION

Chemistry is all about how atoms and molecules interact with themselves and each other resulting in properties and phenomena that can be detected and observed at the macroscopic scale. It follows quite closely then, that an important goal of chemistry education is to help students understand how macroscopic phenomena are governed by interactions and energy changes that accompany changes in interactions at the molecular level. While recent works on large-scale curricular reforms to support students in this goal have many origins, nearly all such efforts view energy as central to teaching, learning, and understanding chemistry (Cooper & Klymkowsky, 2013a; Dukerich, 2015; National Research Council, 2012; NGSS Lead States, 2013; Talanquer, 2013). Furthermore, energy has been identified as both a core component of chemistry, and the sciences in general (National Research Council, 2012, Ch. 3), and a lens through which phenomena can be investigated (National Research Council, 2012, Ch. 4).

Despite the emphasis that disciplinary experts and curriculum designers place on the importance of energy, reports of student difficulties related to energy concepts are widespread (Boo, 1998; Cooper & Klymkowsky, 2013b; Nilsson & Niedderer, 2014; Özmen, 2004; Sozbilir, 2002; Teichert & Stacy, 2002). Recently, research has begun to focus less on ways that students have incorrect understanding of content (often referred to as misconceptions) and more toward describing the ways that students coordinate their understanding of content, almost always in the context of how that knowledge can be used (Becker & Cooper, 2014; Becker, Noyes, & Cooper, 2016; Becker, Rupp, & Brandriet, 2017; Brandriet, Rupp, Lazenby, & Becker, 2018; Cooper, Corley, & Underwood, 2013; Cooper, Kouyoumdjian, & Underwood, 2016; Cooper, Underwood, Hilley, & Klymkowsky, 2012;

Cooper, Williams, & Underwood, 2015; Kararo, Colvin, Cooper, & Underwood, 2018; Williams, Underwood, Klymkowsky, & Cooper, 2015).

One approach to supporting student learning of concepts with which students have been shown to have difficulty is the learning progression approach. Learning progressions are research-based descriptions of how students' knowledge and sophistication of a big idea builds over time (Stevens, Delgado, & Krajcik, 2010). Importantly, learning progressions describe not just what students should know, but also what students should be able to *do* with their knowledge, describing how sophistication of understanding increases as evidenced by students' ability to show their knowledge in use (National Research Council, 2012).

Previous work in the Cooper group has developed a learning progression describing how the relationship between chemical structure and macroscopic properties can be organized and leveraged to improve student learning of historically difficult concepts in postsecondary general chemistry (Cooper et al., 2012). Unfortunately, little research has been published that describes how energy can be systematically treated in a similar manner to support student understanding across the general chemistry curriculum at the undergraduate level.

The current work is a continuation of previous work describing how students in a reformed general chemistry curriculum understand relatively simple interactions while explicitly addressing the role of energy as interactions are formed or overcome (Becker & Cooper, 2014; Becker et al., 2016). This research is focused on how students understand the process by which an ionic solute dissolves in water to form an aqueous solution and explain an observable macroscopic temperature change that accompanies solution formation.

There were three primary phases of this research. In the first phase, described in Chapter 4, students were interviewed to elicit their understanding of how macroscopic observable energy changes could be explained by changes in interactions and energy transfer at the atomic-molecular level across a variety of contexts. The solution formation portion of these interviews was then analyzed to generate themes describing successes, difficulties, and strategies for success. These findings were used to inform the development of a new formative assessment activity including two research assessments: the Solvation Representation Assessment (SRA) and the Thermal Energy in Solvation Assessment (TESA).

Chapter 5 describes the second phase, in which students' drawn representations of solutions and the solvation process were analyzed to characterize how the drawings indicated students' understood the mechanism by which solutions are formed. This study contained four research questions (RQs):

RQ 1: How do students represent fully dissolved solutions of ionic salts?

RQ 2: How do students represent the mechanism of the solution process?

RQ 3: What aspects of the task prompt are effective at eliciting evidence of student understanding?

RQ 4: How does the context of the task prompt (formative vs summative) affect student responses?

To address these questions, sample populations from three semesters were selected, allowing for comparison between an initial prompt and the revised SRA (in fact two groups of SRA, an initial group and a replication group) as developed following interviews. Students' use of interactions in representations of partially- and fully dissolved systems was then compared across assessment version (initial and SRA), stage of solvation (partially and fully dissolved), and assessment type (formative and summative assessment). Results of these analyses provide implications for assessment design in general, in addition to specific goals for future teaching and formative assessment design.

Student explanations of the temperature change that accompanied solution formation were studied using the TESA in Chapter 6. Similarly to before, explanations were analyzed to characterize students' mechanistic understanding of the solution formation process. Two research questions framed the analysis of student explanations:

RQ 1: How do students use ideas of interactions while explaining a temperature change?

RQ 2: What aspects of the task prompt are effective at eliciting evidence of student understanding?

Analysis of student explanations of the temperature change was informed by the desire to understand why students were less successful representing interactions in partially dissolved than in fully dissolved portions of the SRA. Analysis focused on formative assessment responses to characterize the way students understood these phenomena as they developed their understandings. Three versions of the explanation prompt were used in this research (initial, TESAv1, and TESAv2); one sample from each version was selected to address the research questions. Students' use of interactions in explanations was characterized and compared among the three versions to see if the way students used interactions was different based on the explanation prompt. To address research question 2, responses to explanation prompts were compared to use of interactions in the partially dissolved portion of the SRA. Organizing analysis in this way allowed me to investigate whether any explanation prompt resulted in more use of interactions *relative to students' response to the SRA*. Results from this research include implications that about how students successfully include components required to demonstrate mechanistic understanding and further implications pertaining to assessment design.

While students' responses were characterized and evidence of mechanistic understanding was observed, the most generalizable results of this research concern the importance of careful design of assessments, including the need to ensure that assessments are capable of eliciting evidence of understanding before concluding that lack of success is evidence of absence of understanding.

CHAPTER 2 — THEORETICAL FRAMEWORKS

How do students learn, and how can we support them?

Most educators agree that as we learn we construct our knowledge, and in that process our prior knowledge, the situations in which knowledge is constructed, and the purpose for which that knowledge is used – referred to as a whole as Meaningful Learning – are critical to the development of coherent useful knowledge (Novak, 1977; see also Bretz, 2001). It is proposed that new information that does not meet these three criteria will not be well connected to the learner's prior knowledge and result in fragmented understanding or difficulty applying that information to new contexts.

This is particularly problematic in chemistry because of the multiple ways that content may be represented. Johnstone (1982) noted the ease with which expert chemists are able to switch contexts from descriptive and functional, to representational, to molecular while noting that any explanatory power lays exclusively in the molecular scale. Further complicating the ability of learners to make connections between new chemistry content and their prior knowledge and experiences is that many ideas in chemistry, especially at the explanatory molecular level, are deeply unintuitive based on our lived experiences in the macroscopic world. I can think of no analogs in the macroscopic world that can be applied to concepts such as quantization of atomic and molecular orbitals, energy levels, or light; the idea that atoms are mostly empty space; all matter is made of particles, and eventually they are not able to be further divided; or that forming interactions *releases* energy.

Traditional chemistry curricula tend to present topics in isolation from each other as each new chapter is covered without making connections that would assist students in organizing this new knowledge to support Meaningful Learning. Because of the difficulty involved in relating potentially unintuitive new content to student's prior knowledge, particularly since the *reason* that new content is learned is not often apparent to the learner, traditional curricula may have the unintended consequence of promoting isolated "knowledge islands" in student's brains – disconnected and ultimately not very useful knowledge that can only be called up when explicitly prompted for that explicit piece of knowledge.

One promising approach designed to help students make connections to the *weird* ideas found in chemistry is to design curricula around core ideas and the connections between them (Cooper, Posey, & Underwood, 2017). This strategy is one of the key components of what the National Research Council (2012)[1] has described as an approach to help "students build the capacity to develop more flexible and coherent—that is, wide-ranging—understanding of science" (National Research Council, 2012, p. 25). Curricula leveraging this design philosophy have been developed for K-12 (NGSS Lead States, 2013) and undergraduate learning environments (Cooper & Klymkowsky, 2013a)

This strategy has been used to help students make connections between atomic-molecular structure and properties (Cooper et al., 2013; Cooper et al., 2012), bonding and interactions (Becker et al., 2016; Cooper et al., 2015; Williams et al., 2015), and energy (Cooper & Klymkowsky, 2013a; Cooper, Klymkowsky, & Becker, 2014; Cooper et al., 2017). By connecting discrete topics to these core ideas students can build a robust network of well-connected concepts and skills that can be used in new situations and contexts.

[1] This reference, titled *A Framework for K-12 Science Education: Practices, Crosscutting Concepts, and Core Ideas* will be referred to as *The Framework* for the balance of this dissertation

Evaluating student knowledge and understanding

The first step to evaluating any curricula or instructional intervention is determining what learners know and can do with their knowledge. As chemists, we see value in being able to understand the world around us by using the previously mentioned atomic-molecular ideas of structure, properties, interactions, and energy. We also appreciate that knowledge is little more than trivia if it cannot be used in a productive way. *The Framework* identifies eight such ways to use scientific knowledge, which they refer to as "Scientific and Engineering Practices"[2], as seen below in Figure 2.1.

PRACTICES FOR K-12 SCIENCE CLASSROOMS

1. Asking questions (for science) and defining problems (for engineering)
2. Developing and using models
3. Planning and carrying out investigations
4. Analyzing and interpreting data
5. Using mathematics and computational thinking
6. Constructing explanations (for science) and designing solutions (for engineering)
7. Engaging in argument from evidence
8. Obtaining, evaluating, and communicating information

Figure 2.1 — Scientific and engineering practices (National Research Council, 2012, Reprinted with permission from The National Academies Press, p. 42)

The *Practices* can be thought of as instances of knowledge in use because their use is contingent on coordination with disciplinary content; that is, asking questions is not a useful exercise if you do not have the knowledge base to understand what constitutes a productive question (Berland et al., 2016). A corollary to this is that if knowledge cannot be

[2] Hereafter referred to as *Practices*

put into use, whether in the context of the formalized *Practices* on in some other context, there is little to be gained by learning.

Assessment principles

Because the key factor to determining whether content has been productively learned is the ability to use that knowledge in a generative way (e.g. situated in a *Practice*), it follows that a learner's understanding can be characterized by her ability to engage that content in a *Practice*.

The general approach used to assess student understanding in the current work, often referred to as construct-centered design, is characterized by defining: (*i*) the "construct", which is what we want students to know and be able to do with that knowledge, (*ii*) how we want students to demonstrate that knowledge, and (*iii*) how students' responses will be evaluated (Mislevy, Almond, & Lukas, 2003; National Research Council, 2001). In practice, an example of this approach designed to characterize student understanding of intermolecular forces might contain the following steps:

(i) Selection of London dispersion forces as the content and predicting relative strength of interactions as the task

(ii) Prompt design, "predict and explain whether a sample of helium or a sample of krypton would have a higher boiling point"

(iii) Choose relevant features of an explanation that would be acceptable evidence that the student understands the origin of London dispersion forces. For example, is referring to "strength of interactions" sufficient? Or is a discussion of size and polarizability of krypton's electron cloud as a causal element because it can generate a larger instantaneous separation

of charges, which can then induce a larger induced dipole in another atom required?

This approach treats student responses to assessment tasks as data that must be interpreted and used to provide evidence about how the student understands the construct. This means that the way that responses are evaluated (step *iii* above) will result in different evidentiary claims about the nature of student understanding and therefore must be carefully considered. The complicated nature of most chemical phenomena implies that there will generally be a wide range of evidence of student understanding generated during this process. This approach also allows for characterization of intermediate levels of understanding, based on evidence obtained from student responses. This last point is important because it allows researchers to track how student understanding changes along a scale from novice to expert-like (Wilson, 2005). This approach provides a method to triangulate student understanding by using different assessment tasks to measure the same construct.

<u>Explanations and Mechanistic Reasoning</u>

In this dissertation the scientific *Practices* of constructing models and explanations will be used to explore and characterize how students reason about the dissolution of ionic compounds in water. Of particular interest is exploring how students understand the mechanism by which this process occurs.

While there are many approaches to defining what constitutes a mechanism (and mechanistic reasoning), most researchers agree (Krist, Schwarz, & Reiser, 2018) that a mechanism has several requirements:

1. A phenomenon that is to be explained by the mechanism

2. Entities or parts that participate in the mechanism
3. A sequence of events that constitute the mechanism
4. The participants involved are at least one scalar level below that of the phenomenon

The last point above, that mechanisms of chemical phenomena require that the entities involved are at least one scalar level below the level of the phenomenon, is crucial. For example, Cooper et al. (2016) observed some students using the Bronsted acid-base model to reason about a reaction of HCl and water (that is, they described it as a proton transfer between an acid and a base), while others used the Lewis model (that is, they invoked the electron pair of the water interacting with the H from HCl). The Lewis model involves entities (electrons) at a scalar level below the Bronsted model, and therefore these students were determined to have provided a more sophisticated causal mechanism for the reaction. This idea was supported by the fact that students who were able to construct causal mechanistic explanations (i.e. they used the Lewis model of acid-base reactions and also described the electrostatic attraction between the acid and base) were also better able to construct mechanistic representations in the more traditional organic chemistry sense of using mechanistic arrows.

Finally, some researchers differentiate between a mechanism, which characterizes how a phenomenon occurs, and a causal mechanism, which also includes why a phenomenon occurs. In the example of the acid-base mechanism above, the description and use of an electrostatic attraction between the acid and the base is what caused the two species to move towards each other so that the lone pair of electrons could be donated from water to the proton.

Representations

Explanation tasks, on their own, may not always provide sufficient evidence that students understand the construct. The *Practice* of developing and using models provides another way for learners to use their knowledge by constructing a representation, such as an atomic-molecular scale drawing of the phenomenon or a mathematical relationship, and using it to make a prediction. In the specific case of constructing molecular level drawings, the *Practice* of modeling provides further opportunities for students to practice linking the macroscopic scale to the molecular (explanatory) scale (Johnstone, 1982).

As mentioned previously, using construct-centered design to generate evidence of student understanding allows the use of different observations (assessment tasks) to provide additional evidence about students' thinking. This approach has been used to characterize students' understanding of intermolecular forces by having them construct representations and explain intermolecular forces in different substances (Cooper et al., 2015). By utilizing both explanation and representation tasks, the authors were able to gather additional evidence that students' understanding of intermolecular forces was more nuanced than if only one type of evidence was obtained.

CHAPTER 3 — REVIEW OF THE LITERATURE ON SOLUTIONS AND SOLVATION

Student understanding of solutions and solvation has been widely studied. Among the main products of this line of research are a number of documented and replicated student difficulties, often referred to as misconceptions, which have been identified across a range of student ages and levels of expertise. These misconceptions have been observed via interview, multiple-choice, free-response, and drawing methodologies (Çalýk, Ayas, & Ebenezer, 2005).

Prior research on student understanding of the solution process

Most documented difficulties have been observed in student responses of fully dissolved solutions. Researchers using free-response drawing tasks have seen that solutions are often not represented at the particulate level by precollege students (Holding, 1987; Prieto, Blanco, & Rodriguez, 1989). Additionally, students often represent solutions as heterogeneous in nature, with particulate representations containing solute at either the top or the bottom of the “solution” (Abraham, Williamson, & Westbrook, 1994; Prieto et al., 1989).

A brief overview of particulate level errors documented in students’ representations of aqueous solutions includes: transformation of the solute into a new compound (and not simply dissociation of an ionic compound into its constituent ions) (Abell & Bretz, 2018; Abraham et al., 1994; Ebenezer, 2001; Ebenezer & Erickson, 1996; Naah & Sanger, 2012; Tien, Teichert, & Rickey, 2007); dissociation of ionic solute into ionic “molecules” (Kelly & Jones, 2007, 2008; Naah & Sanger, 2013; K. C. Smith & Nakhleh, 2011; K. J. Smith & Metz, 1996; Tien et al., 2007); breaking covalent bonds (Abell & Bretz, 2018; Herrington, Sweeder, & VandenPlas, 2017; Naah & Sanger, 2012; K. C. Smith & Nakhleh, 2011; K. J.

Smith & Metz, 1996; Tien et al., 2007); and problems correctly representing the intermolecular forces present (Abell & Bretz, 2018; Ebenezer, 2001; Kelly & Jones, 2007, 2008; K. C. Smith & Nakhleh, 2011). This last difficulty is important, as a number of studies have shown more specifically that students have difficulty representing solutions as containing solvated ions (Abell & Bretz, 2018; Ebenezer, 2001; Herrington et al., 2017; Kelly & Jones, 2007, 2008; K. C. Smith & Nakhleh, 2011; K. J. Smith & Metz, 1996). This is troubling since it is the existence of interactions between the solvent and solute that ensures the solute is able to dissolve in the first place.

While a bulk of the research about students' ability to represent and explain solutions and solvation is focused on student difficulties, some studies have found evidence of student ability to represent many of the important and complicated ideas related to these phenomena. Recall that solutions form via an initial molecular collision (and the subsequently formed interaction) between the solvent and an intact solute so that energy may be added to overcome the interactions holding the solute together (whether those interactions are ionic bonding interactions, as in sodium chloride, or intermolecular forces, as in sugar). Kelly and Jones (2007) investigated the effect of viewing molecular animations on students' ability to represent and explain solvation, using purposeful sampling to select students who were more descriptive on a screening task. While none of the students included interactions between the solvent and intact solute before viewing the animations, afterwards 7 of 18 participants drew or wrote about solvent molecules pulling ions from an intact solute. K. C. Smith and Nakhleh (2011) reported evidence that some students viewed the solvation process at the mechanistic level since they referred to collisions as necessary to supply the energy needed to overcome ionic bonding interactions in the solute during interviews. More recently, Abell and Bretz (2018) observed students describe interactions between water and ions in an intact solute as necessary to cause formation of aqueous solutions of ionic salts.

Another aspect of student representations that has been noted is the presence of interactions between the solvent and individual solute particles (*i.e.*, solvated ions or particles, or spheres of hydration). While these findings are rarely the primary focus of research on this subject, they have been explicitly noted in interview (Abell & Bretz, 2018; K. C. Smith & Nakhleh, 2011) and intervention settings (Bruck, Bruck, & Phelps, 2010; Ebenezer, 2001; Kelly & Jones, 2007; Tien et al., 2007). Specifically, improvement in students' use of representations of solvation spheres in solutions has been seen resulting from interacting with animations (Ebenezer, 2001; Kelly & Jones, 2007) and laboratory activities (Bruck et al., 2010; Tien et al., 2007). Though these studies show that students are capable of representing solutions as being composed of solvated ions, the difficulty of this task is reinforced by results of a follow-up study published by Kelly and Jones (2008). While 14 of 18 students included solvation spheres in their drawings of dissolved sodium chloride after viewing the animation in the original study (2007), none of them did so when drawing reactant solutions in the follow-up study (2008). Furthermore, half of the representations from the follow-up study included ionic pair representations of sodium chloride.

Prior research on student's understanding of solutions, thermochemistry, and thermodynamics

There has been considerably less research about how students understand, explain, or represent how energy might be related to the solvation process or solutions in general.

As with solutions and the solvation process, most published results primarily focus on student difficulties.

Early research observed that secondary school students often had understanding of solutions and related phenomena (such as evaporation and the dissolving process itself) that did not consider energy at all (Nusirjan & Fensham, 1987).

Ebenezer and Fraser (2001) interviewed undergraduate students to elicit their understanding of energy changes that accompany dissolution. While the authors explicitly mention analysis of the process of dissolving, including a reference to pulling apart electrostatic attractions, their conclusions were primarily described in terms of the direction in which students described energy flow. Students were found to have a variety of conceptions about where and how energy flowed in three different examples (mildly endothermic, highly exothermic, and highly endothermic). Inconsistencies in students' reasoning were noted, both in reasoning between examples and in operational definitions of concepts, and a set of instructional strategies intended to remediate student difficulties was generated.

In work published in 2003, Greenbowe and Meltzer analyzed student responses to thermochemistry exam questions. Most of their findings described mathematical errors observed in students' answers (such as sign confusion, incorrect usage of equations, or confusing temperature change and heat). However, a few of their findings were more relevant to the current research. The first was related to student ability to identify system and surrounding in a calorimetry question. Of the 207 responses, only 22% and 6% correctly identified the system and surroundings, respectively. Additionally, the authors observed seven categories of incomplete or incorrect characterizations of the system and six such categories for the surroundings. They also reported a student's treatment of energy as something transferred between and amongst *chemical species* (similarly to how two conductive objects at different temperatures will transfer heat) rather than being absorbed or evolved as a consequence of overcoming or forming interactions.

More recently, Abell and Bretz (2018) investigated general chemistry and upper-level undergraduate students' understanding of dissolving and precipitation in the context of solution thermochemistry. They observed that only eight of thirty-two students correctly and consistently described the energy flow required for interactions and bonds to break or form across four examples of endothermic and exothermic processes in an interview setting.

Also in 2018, Bain and Towns conducted a similar set of interviews with general chemistry, organic chemistry, upper-level undergraduate, and physical chemistry graduate student participants. Their study additionally expanded the scope of examples to include endothermic and exothermic chemical reactions in addition to an endothermic dissolution. In their analysis, the authors observed distinct patterns in reasoning used by students related to themes of state functions (enthalpy, entropy, and Gibbs energy), temperature changes, and teleological reasoning. Schemas of reasoning for the state functions were described as having a range of complexities, from surface-level to multi-faceted and interconnected. In addition to investigating entropy and spontaneity in the context of student reasoning about and explanation of processes with macroscopically observable temperature changes reactions, this research is particularly important in two important ways. First, it purposefully included participants across a wide range of the novice-expert continuum, from undergraduate general chemistry to third year physical chemistry graduate students. Second, this is the only study I have found that combines a high level of participant expertise, focus on chemical processes with macroscopic observable temperature changes, and is not merely descriptive in nature, but is generative with respect to analysis of participants' reasoning.

Concluding remarks

Chemistry is unique among the physical sciences in that providing a causal explanation of a property or phenomenon *requires* coordination of many concepts across a vast range of scales. It is the need to translate across scales, using atomic-molecular level models and entities to provide explanations for macroscopic phenomena that makes chemistry uniquely difficult. Furthermore, our macroscopic understandings of how the world works do not translate to the molecular world; explanations at the molecular level are complex and often counterintuitive. It is not surprising then, that a great deal of research on student understanding tends to focus on documenting the kinds of problematic non-normative ideas, sometimes referred to as misconceptions, that often emerge from studies.

It is clear that the literature describing student understanding of solutions and solution formation is no different, with the predominant focus having been documenting the many aspects of solutions and solution formation processes that are difficult for students to explain or represent. Because of the focus on student difficulties, there are numerous reports of, for example, students representing the dissolving process as a phase change, a chemical reaction with water, or resulting in breaking covalent bonds.

Looking at this literature, most of the research findings can be described as either (*i*) cataloging misconceptions and difficulties observed in student reasoning or (*ii*) characterizing the potential effects of a short-term instructional intervention. This has resulted in us knowing a great deal about student difficulties, but relatively little about how to help students develop more robust and useful understanding of the molecular level process and mechanism by which solutions form; what is largely missing from the literature is a way to characterize and support student's conceptions of solutions and solvation that captures a range of understanding.

CHAPTER 4 — RESEARCH SETTING AND DEVELOPMENT OF RESEARCH ASSESSMENT ITEMS

There are two principle components of the research setting in which this dissertation is situated: a transformed general chemistry curriculum *Chemistry, Life, the Universe and Everything* (CLUE) and a formative assessment activity designed to support and scaffold student explanations of enthalpic and entropic changes that accompany formation of an aqueous ionic solution. This chapter first introduces the CLUE curriculum, describes its implementation at Michigan State University (MSU), and gives a description of how solutions are treated in text, lecture, and recitation contexts. The rest of the chapter describes technical aspects of this research, including how and when data was collected and how the assessment items were developed.

Chemistry, Life, the Universe and Everything

Description of the Learning Environment

The research presented in this dissertation is embedded in a transformed general chemistry curriculum, *CLUE*, as implemented at MSU. CLUE is an evidence-based reform effort that has been designed around four interrelated core concepts of chemistry: electrostatic and bonding interactions, atomic-molecular structure and properties, change and stability in chemical systems, and energy (Cooper & Klymkowsky, 2013a; Cooper et al., 2017). By focusing on these core ideas and making explicit the connections among them across a variety of chemical systems from simple (the interaction of noble gases) to complex (coupled biological reactions), CLUE seeks to help students develop an understanding of chemical phenomena and the mechanisms by which these processes occur that treats these core ideas as causal. Furthermore, the development of CLUE has leveraged a design based research strategy (Brown, 1992) of iterative design-assess-revise-assess cycles, of which this research is a part.

As enacted at MSU, the CLUE curriculum consists of lecture (meeting either thrice weekly for 50 minutes or twice weekly for 80 minutes) and recitation (weekly 50 minute periods) sessions. Lectures feature frequent student-student and student-teaching assistant interactions, typically highlighting prediction or explanation tasks coupled with an anonymous interactive student response system (iClickers). In addition to these short discussion periods, students periodically engage with more in-depth activities exploring central theories, phenomena, or concepts. In weekly recitation periods students work in small groups to complete worksheets prompting them to predict, explain, draw representations, and support arguments to complete formative assessment tasks relating to content from the lecture. Teaching assistants facilitate these meetings as necessary by asking probing questions to assist students in constructing their understanding in a low-stakes learning environment.

Homework assignments utilize the beSocratic system (Bryfczynski, Pargas, Cooper, & Klymkowsky, 2012). This online platform enables the creation of activities, which can include free-form student drawing, graphing, multiple choice, and free-response text input. Context-specific feedback can be programmed into graphing, drawing, and multiple-choice items. Throughout the course, generally after each lecture, homework assignments were administered via beSocratic and submissions were graded for completion. Feedback was provided through in-class discussion, the previously mentioned programmed context-specific feedback, or both. I specifically note that, while homework activities are reviewed in lecture, students are *not* provided written answers to these tasks.

Treatment of Solutions and Solvation in the CLUE Curriculum

The treatment of solutions and solvation in CLUE leverages repeated explicit references to connections among molecular structure and properties, interactions, energy, and stability and change across contexts to support students' ability to use their understanding to predict, explain, or engage in arguments from evidence for a wide range of phenomena. These frequent explicit references to core ideas allow students to connect new material to their prior knowledge in a way that contextualizes and facilitates learning. Previous work has shown that students in the CLUE curriculum are particularly well equipped to draw and use structures to make predictions about properties (Cooper et al., 2012). Instruction on solutions occurs in the second semester (subsequently referred to as "GC2") and builds upon this foundation by explicitly drawing on students' understanding of interactions and intermolecular forces and extending them to more complicated systems as described below.

Text

The CLUE textbook is different from typical general chemistry textbooks in that it is not intended to be a "one stop shop" containing anything a student might want to know about the class content. It is instead intended to be "readable and engaging" (Cooper & Klymkowsky, 2017), and provide context to help drive the narrative of the course from topic to topic, focusing on the core ideas and how they relate to both new and previously covered material. The solutions chapter begins by recalling topics previously covered, calling attention to atomic and molecular structure, interactions of atoms and molecules, and how thermodynamic changes can lead to phase changes.

The concept of a solution is then introduced and defined, beginning with solutions of two liquids using the example of ethanol in water. The reader is reminded that ΔG is negative for thermodynamically favored processes, but that the relationship of enthalpy and entropy to Gibbs free energy implies that either enthalpy *or* entropy could cause solution formation to be favorable.

Solubility is explained as a continuum to explore why some substances form solutions while others do not. Illustrative examples include a variety of compounds including alkanes, alcohols, ethers, a diol, and glucose with the observation that molecules with hydroxyl groups are more soluble in water than those without, and that for any particular functional group, molecules with fewer carbons are more soluble than molecules with more carbons.

The process of solvation in water is then probed more deeply, explaining that for a substance to dissolve in water the interactions holding that substance together must be replaced by interactions with water. Diamond is used as an example to link this idea to previous content (the structure of diamond as a covalent network solid). Diamond does not dissolve in water because its covalent bonds are stronger than the interactions its carbon atoms could form with water. The observation is made that substances with more hydroxyl groups are more soluble in water because interactions between the water molecule and the hydroxyl group are similar to the interactions that water has with other water molecules, which are hydrogen bonding interactions.

Entropic effects are introduced with the example of oil and water not being miscible. If oil were to dissolve in water, water would maximize its hydrogen bonding interactions with itself since those interactions are much stronger than the interactions between water and oil molecules. This extended network of hydrogen bonding interactions would actually reduce the entropy of the water molecules, and because the entropic contribution of dispersing oil molecules is $\sim\Delta H = 0$, the overall ΔG would be positive (recalling that $\Delta G = \Delta H - T\Delta S$), so the oil does not dissolve in water.

The next topic covered in the text is the solubility of ionic compounds. It is noted that ionic bonding interactions are strong, but the reader is aware that sodium chloride dissolves in water. How can these opposing ideas be reconciled? A snapshot of a molecular level animation showing water molecules hydrating a sodium ion from the surface of the crystal is shown, and the reader is reminded to consider the system as a whole and include the interactions that form between ions and water.

It is noted that when they dissolve, some salts cause the temperature to increase while others cause the temperature to decrease. Using the example of calcium chloride, a salt that causes the temperature to increase when it dissolves, the interactions that are present before and after solution are identified, and the ions and their respective solvation shells are identified as the system. Once the system has been identified, the rest of the solution is the surroundings, and if the solution increases in temperature that must mean that the energy came from the system. Because the system released energy, it follows that the interactions in the system after the solution has formed are stronger than the interactions before the solution was formed. The reader is then reminded that when sodium chloride dissolved that the temperature decreased. This means that since the system required an input of energy (which came from the surroundings, i.e., the rest of the solution) that the process of sodium chloride dissolving is an *entropically* driven process. It is pointed out that many solvation processes have unfavorable enthalpic contributions, which means that entropic contributions can be quite important in determining whether a substance will dissolve.

Final topics covered in the text include how larger molecules, specifically biomolecules, can have multiple properties; how the formation of micelles by amphipathic molecules can be explained by differing solubility of different parts of molecules; the effect of temperature on solubility; and solutions of solids in solids using alloys of metals as examples. The chapter on solubility and solutions closes by asking the reader if solution formation is a reaction. The examples of ethanol in water and sodium chloride in water are used to show that this is a more complicated question than it might initially seem. A final example of dissolving HCl(g) in water leads in to acid-base reactions and the next chapter.

Lecture

A typical CLUE lecture includes frequent opportunities for students to discuss concepts amongst themselves, with a teaching assistant, or with the instructor. These opportunities are usually in the context of responding to a formative assessment task, such as responding to a clicker question or drawing a representation of a phase change at the atomic-molecular level. The organization and content during two lecture periods covering solutions, solvation, and thermodynamic factors affecting solubility are described below.

Lecture coverage of solutions begins similarly to the text, where solutions are introduced, defined, and compared to mixtures. An example of dye mixing in water is shown, which leads to a discussion of whether the mixing process is reversible, especially considering the positional entropy of dispersed dye molecules. Students are then asked a series of clicker questions about what types of substances dissolve in water (e.g. – diamond, sugar, oil), and are then shown a molecular-level animation of what happens when sodium chloride dissolves in water.

Students are asked to come up with some factors affecting solubility; it is anticipated that they will mention something about the solvent and the solute (and the types of interactions, bonding, or intermolecular forces present), entropy change, and temperature. Students are then asked another series of clicker questions regarding the energy change of the changes that must occur for a solute to dissolve: (*i*) interactions between solute particles must be overcome, (*ii*) some interactions between solvent particles must be overcome, and (*iii*) new interactions formed.

Next, a table comparing the molar mass of propane, ethanol, and dimethyl ether is shown. Students are asked to predict the most and least soluble (in water), while considering the factors that affect solubility. To further link solubility to interactions, students are asked to draw structures of the three molecules, and show how each of them would interact with water. For another example, students are asked to consider ethanol, butanol, hexanol, and 1,6-hexanediol and again think about the structural features that affect solubility.

The first example of a solid students are asked to make predictions for is sucrose. Its structure is shown, and student are asked what intermolecular forces they predict between sucrose and water with the intention that they will notice the many polar hydroxyl groups and think of the hydrogen bonding interactions that can form. A molecular-level animation of what happens when sucrose dissolves in water is then shown.

The second lecture begins with the example of calcium chloride dissolving in water, an example of a process in which the temperature increases when the solution is formed. In addition to describing the example, plastic bags containing solid calcium chloride and water are distributed to students so that they can feel the temperature change. Students respond to clicker questions asking them to predict the signs of ΔG and ΔH for the solvation process they experienced in the plastic bags. The atomic-molecular animation of the solvation of sodium chloride is shown again; students are prompted to think about how interactions are changing throughout the solvation process. Students then answer a clicker question asking them to compare the strength of interactions in the solution to those in the separated solute and solvent based on the observed increase in temperature. Students are then asked to draw (*i*) a picture of solid calcium chloride, clearly showing the forces holding the solid $CaCl_2$ together and (*ii*) a picture of aqueous calcium chloride. Students are encouraged to discuss their representations with each other. The instructor and teaching assistants are circulating through the lecture hall to answer or ask questions to help students draw representations of calcium chloride in these two states. At the end of the exercise students are asked what forces are present in aqueous calcium chloride and what they can say about the relative strengths of the forces. Once students have had time to complete these tasks, the instructor asks the class what interactions were present before and after solution. After constructing representation and discussing the interactions present before and after solution, students then answer the same clicker question as before asking them to compare the strength of interactions in the solution to those in the separated solute and solvent based on the observed increase in temperature. Over the course of more clicker questions, students are asked to predict the sign of ΔS (because the solvation of calcium chloride is exothermic, there was actually not enough information to predict ΔS) and then determine whether the sign of ΔG, ΔH, or ΔS indicated whether a substance is soluble.

Following the example using calcium chloride described above, students were given plastic bags containing solid ammonium chloride and water so that they could feel an example of an endothermic solvation process. Students were asked the same series of clicker and discussion questions as for calcium chloride, and also drew representations of ammonium chloride as a solid and as an aqueous solution. Once students have had time to complete these tasks the instructor then asks the class what interactions were present before and after solution for ammonium chloride. The interactions present for ammonium chloride are compared to the previously discussed interactions present for calcium chloride. Students are asked to explain why the solvation of calcium chloride is exothermic and the solvation of ammonium chloride is endothermic since they both have similar sets of interactions before and after dissolving, anticipating that students will notice the higher charge of the calcium ion (compared to the ammonium ion) and connect this higher charge to the formation of stronger interactions with water, therefore causing energy to be released to the surroundings to be observed as an increase in temperature of the solution.

Over the course of more clicker questions, students are asked to predict the sign of ΔS (because the solvation of ammonium chloride is endothermic, there *is* enough information to predict ΔS this time) and then determine whether the sign of ΔG, ΔH, or ΔS indicated whether a substance is soluble.

To end the lecture, an insoluble salt (calcium oxide) is presented with the information that ΔH for solution of CaO is about zero. Students then answer clicker questions about the sign of ΔG (zero, because it is insoluble) and ΔS (mathematically must be negative) and are asked to think about why the entropy would decrease. It is pointed out that calcium oxide would dissociate into highly charged Ca^{2+} and O^{2-} ions, and that these small highly charged ions actually attract the water molecules so strongly that they are effectively locked into solvation shells around the ions. This strong attraction partially immobilizes some of the water molecules, resulting in a decrease in entropy such that the process is not thermodynamically favorable. Later lectures extend the idea of entropically driven processes (such as the insolubility of CaO above) to hydrophobic effects and the temperature dependence of solubility of solids and gasses.

Recitation

Recitations are used to provide students with an environment where they can practice using and constructing their knowledge to make predictions, provide explanations, construct arguments from evidence, and construct models in groups of three or four to complete a worksheet containing questions related to content presented in lecture. The worksheet covering solutions and solvation is shown below in Figure 4.1.

1. For each solute, and solvent indicate what interactions are present in each substance, and what interactions are present between the solute and solvent in solution. (Draw two or more structures in each box showing interactions). DO you predict that the solute is soluble in the solvent?

Solute	Solvent	Solution	Soluble?
CH_3OH	H_2O		
CH_3OH	CH_3COOH		
$NaNO_3$	H_2O		

Solute	Solvent	Solution	Soluble?
$CaCl_2$	Hexane (C_6H_{14})		

2. Hexanol ($CH_3CH_2CH_2CH_2$ CH_2CH_2OH) is insoluble in water to any great extent, but 1,6-hexanediol ($HOCH_2CH_2CH_2CH_2$ CH_2CH_2OH) is soluble. Draw pictures to explain why this so.

3. Calcium phosphate ($Ca_3(PO_4)_2$) is insoluble in water. The ΔH for solution is about zero. Predict the signs of ΔS and ΔG, and explain your reasoning by drawing molecular level pictures.

Figure 4.1 — Recitation worksheet for solution and solution formation

Task 1 on the worksheet has students draw interactions for a variety of substances, including methanol, water, acetic acid, sodium nitrate, calcium chloride, and hexane. Students are also asked to draw representations of solutions formed when substances are mixed together and predict whether each solute would be soluble in the solvent it was paired with. The intention is for students to identify the strong intermolecular forces present for the first three solute solvent pairs (hydrogen bonding, hydrogen bonding, and ion-dipole interactions, respectively) and predict that the solute would be soluble. For the last pair, calcium chloride and hexane, hopefully students identify London Dispersion Forces as the only intermolecular forces present and therefore predict that calcium chloride would not be soluble.

Task 2 instructs students to explain the difference in solubility, in water, of hexanol and 1,6-hexanediol and support their explanation with atomic-molecular level representations. Because students are told that hexanol is not soluble, a complete response will depict hydrogen bonding interactions between the water and single hydroxyl group of hexanol and between water and both hydroxyl groups of the diol. Explanations will state that the fewer possible hydrogen bonding interactions for hexanol mean that there is not sufficient interaction with water molecules for hexanol to be soluble. A more complete explanation would also mention that water molecules would maximize their hydrogen bonding interactions with other water molecules because of the weakness of the London Dispersion Forces between the hydrocarbon end of hexanol and water, which would result in a negative entropy change. Because ΔH for dispersing hydrocarbons is approximately zero, the overall ΔG for this process would therefore be positive, resulting in hexanol not being soluble in water.

Task 3 is another explanation task that additionally explicitly prompts students to consider enthalpic and entropic factors in their response. A successful response will represent calcium phosphate as isolated Ca^{2+} and PO_4^{3-} ions individually interacting with water molecules. Due to the high charges on the calcium and phosphate ions, the interaction with water molecules will be quite strong, and the ions will partially immobilize many water molecules (which could easily be represented by showing multiple hydration spheres immobilized at each ion), resulting in a negative entropy change. Because $\Delta H \sim 0$ for this process, that means that the ΔG must be positive, indicating that calcium phosphate is not soluble in water.

Other solution topics in the CLUE curriculum

Additional topics and applications of solutions beyond those described above include further discussion of the entropic origin of hydrophobic effects. Micelle and lipid bilayer formation, how soap works to remove grease, how febreeze isolates and removes odors, and why proteins fold are discussed to provide context to the many phenomena that are entropically driven. Alloys of metals are introduced as examples of solutions of solids in solids. The final topic in this chapter addresses temperature and its effect on solubility. Temperature effects are explored for solubility of solids and gases in liquids, and the differing effect of temperature on solubility of solids and gases is discussed.

Data Collection

The overarching goal of this research is to elicit and characterize student understanding of the sequence of events necessary for an ionic salt to dissolve in water including (*i*) how interactions must be formed or overcome and (*ii*) any relevant energy change, transfer, or transformation. Because there are two components required to demonstrate understanding of the solvation process, any attempt to probe students' understanding must elicit evidence relevant to both components (Mislevy, Almond, et al., 2003; National Research Council, 2001).

To address these components, assessments have been developed in the course of this research that prompt students to (*i*) draw the solvation process at the atomic-molecular level and (*ii*) explain why a given observable temperature change might accompany the solvation process. These two assessments are referred to as the Solvation Representation Assessment (SRA) for the drawing task and the Thermal Energy in Solvation Assessment (TESA) for the explanation task.

Data used in this research was collected from second semester general chemistry (GC2) students enrolled at MSU across multiple semesters. A timeline of research and assessment activities is shown below in Figure 4.2, the development of which is described below in detail. Analysis of the assessments used in this research is described in Chapter 5 (for the SRA) and Chapter 6 (for the TESA).

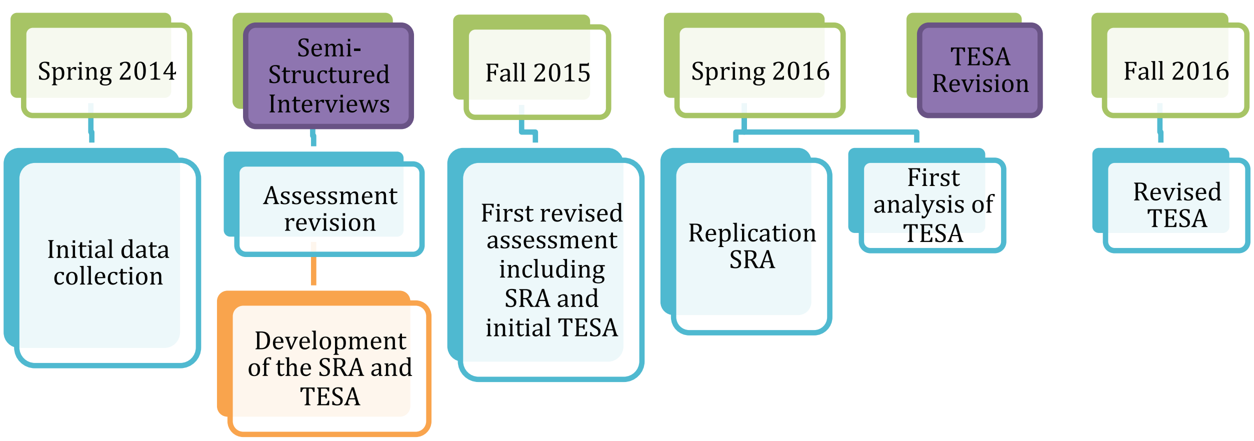


Figure 4.2 — Timeline of assessments implemented in this dissertation

The first phase occurred during the Spring 2014 semester and used formative and summative assessment tasks developed specifically for use in the CLUE curriculum prior to the current research. The formative assessment was situated in a larger formative assessment activity designed to support students as they explained a macroscopic temperature change that occurred as a solution was formed. The summative assessment tasks were administered as a portion of the medterm exam given to students after covering the material in lecture, recitation, and homework.

Following initial analysis of student assessment responses from the Spring 2014 semester, interviews were conducted to probe student understanding of macroscopic energy changes resulting from physical and chemical processes. These interviews were then analyzed with the primary goal of providing a strategy to revise the formative and summative assessments used in the first phase.

In Fall 2015, an initial version of the TESA and the final version of the SRA were first administered. The SRA is still in use as a formative assessment in the CLUE curriculum without modification. Initial analysis of student responses to the TESA led to further revision; the final version of the TESA has been in use as a formative assessment in the CLUE curriculum since Fall 2016.

Participant Population

Student participants were selected from a population of second semester general chemistry students enrolled in the CLUE curriculum at Michigan State University. Over the course of this research (2013-2018), there were approximately 39000 undergraduate students enrolled at MSU per academic year. Gender, ethnicity, and international status demographics are compiled in Table 4.1 below (Michigan State University Office for Inclusion and Intercultural Initiatives, 2018).

Table 4.1 — Michigan State University undergraduate student demographics from 2013-2018

Demographic	13-14	14-15	15-16	16-17	17-18	Average
Male	49.8%	49.8%	49.6%	49.4%	49.5%	49.6%
Female	50.2%	50.2%	50.4%	50.6%	50.5%	50.4%
Black	7.6%	7.7%	8.0%	8.0%	8.3%	7.9%
Asian	4.8%	5.0%	5.4%	5.7%	5.9%	5.4%
Hispanic/Latino/a	4.1%	4.4%	4.6%	4.8%	5.0%	4.6%
Total students of color	19.6%	20.6%	21.5%	22.3%	23.0%	21.4%
White	79.1%	78.3%	77.4%	76.8%	76.2%	77.6%
Domestic	87.4%	86.3%	86.5%	87.2%	88.2%	87.1%
International	12.6%	13.7%	13.5%	12.8%	11.8%	12.9%
Total undergraduate enrollment	37988	38786	39143	39090	38996	38801

At MSU, the CLUE curriculum is implemented in a two-semester large-enrollment general chemistry sequence intended for non-chemistry STEM majors. Other general chemistry sequences housed in the chemistry department are maintained for chemistry majors and honors students. Coenrollment in a general chemistry laboratory course is not required for either semester of CLUE.

As previously mentioned, solutions are covered in the second semester of the CLUE curriculum. As the second of a two-semester course sequence, GC2 has an average spring ("on-sequence") enrollment of 900 students and an average fall ("off-sequence") enrollment of 400 students; approximately 35% of students progress from first to second semester general chemistry at MSU. Overall demographics of students enrolled in GC2 from 2014 to 2018 are shown below in Table 4.2 and compared to overall undergraduate student demographics from the same time period; chi-square analysis was performed for each demographic category to produce the *p*- and Cramer's V values listed.

Table 4.2 — Demographics of students enrolled in GC2 at MSU from 2014-2018; demographics of all undergraduate students at MSU included for comparison

Demographic	GC2	All Undergraduate Students	*p*-value	Cramer's V
Male	44.1%	49.6%	**<0.001**	**0.036**
Female	55.9%	50.4%		
Black	6.5%	7.9%	**<0.001**	**0.055**
Asian	8.4%	5.4%		
Hispanic/Latino/a	4.0%	4.6%		
Total students of color	32.0%	21.4%		
White	67.1%	77.6%		
Domestic	91.2%	87.1%	**<0.001**	**0.040**
International	8.8%	12.9%		
Total GC2 enrollment	5300			

The demographics of students enrolled in GC2 are not equivalent to those of all undergraduate students enrolled at MSU over the time period of this research. There are significantly more females, domestic students, and students of color enrolled in GC2 than in the general undergraduate enrollment. However, the effect size of each of these associations between demographic category and population, as given by Cramer's V, is no larger than 0.055, which indicates very small practical significance (Cohen, 1988).

The 2013-2014 academic year was the first implementation of the CLUE curriculum at a MSU. The first course of the CLUE sequence was taught as one of six lecture sections of first semester general chemistry offered in Fall 2013 (the other five lecture sections used a traditional curriculum); CLUE GC2 was one of two lecture sections of second semester general chemistry offered in Spring 2014. Because this was the first implementation of CLUE in a new environment (initial development of the CLUE curriculum took place at Clemson University), special care was taken to ensure that students were able to enroll in both semesters of the CLUE sequence. Announcements were placed in online course registration listings and academic advisors were requested to suggest that students register for both semesters of the CLUE sequence when possible.

In the Fall 2014 semester, CLUE was taught in two of six lecture sections offered. Again, announcements were placed in online course registration listings suggesting students only enroll in CLUE sections if they were also enrolling in the second semester course. By Spring 2015, all CEM 141 and 142 general chemistry courses used the CLUE curriculum; Fall 2015 was the first time that second semester CLUE was taught "off-sequence". As previously mentioned, Spring 2016 was the first time the final SRA (described in detail below) was administered to students in an "on-sequence" second semester CLUE course. The TESAfinal was first administered in Fall 2016.

Activity development and revision

Multiple versions of two assessments were used to collect the data analyzed in this dissertation. These assessments were situated in a larger formative assessment activity that was designed to support students as they explained a macroscopic temperature change that occurred as a solution was formed. As mentioned previously, formative assessments in CLUE are administered online in the *beSocratic* system, which allows students to produce free-form drawn and written responses (Cooper, Underwood, Bryfczynski, & Klymkowsky, 2014).

<u>Original formative assessment activity</u>

The previously developed formative assessment activity had two main parts. The first dealt with atomic-molecular level representations of sodium chloride before (Figure 4.3a) and after (Figure 4.3b) the solution process. Students were then asked to choose a statement that best described the relative strengths of interactions given the endothermic nature of the solution formation process. Finally (Figure 4.3d), they were asked to draw a representation of how energy might be transferred between the system and surroundings and to explain why the temperature decreased.

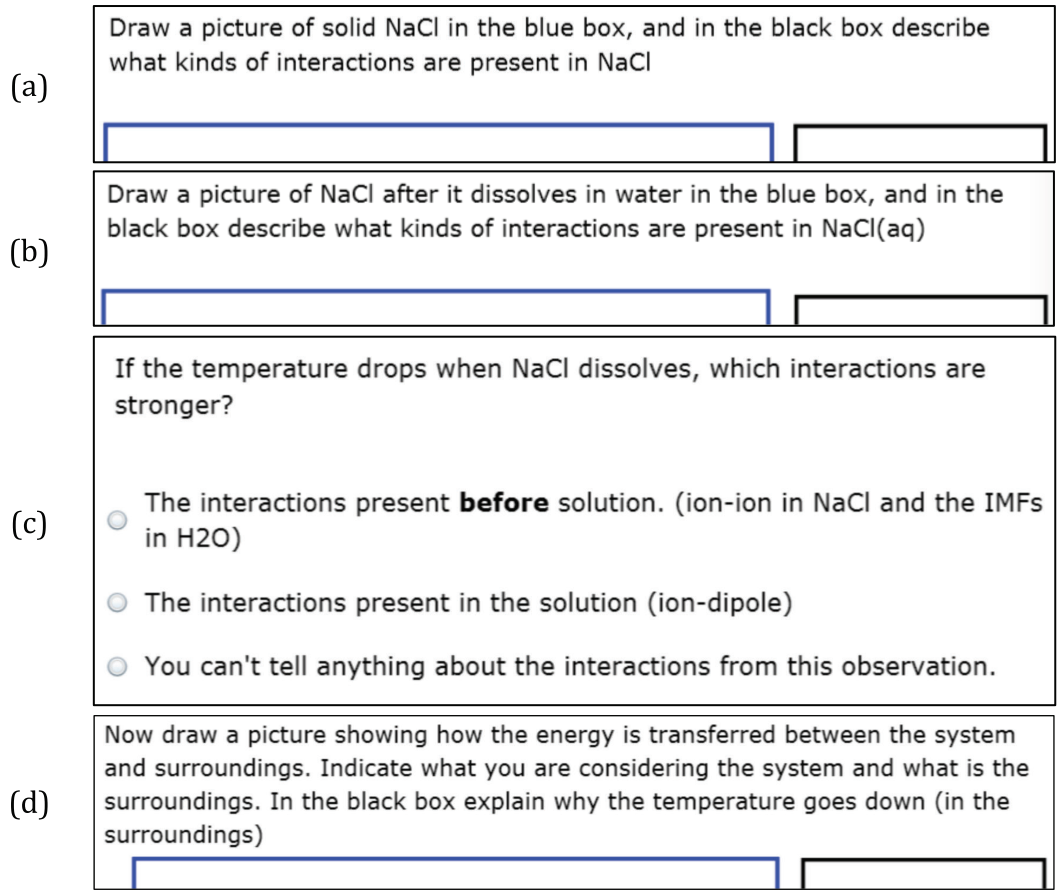


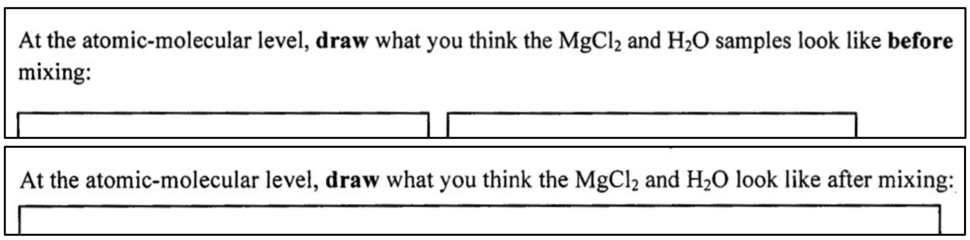
Figure 4.3 — Tasks from first section of initial solvation formative assessment activity. Students were prompted to draw representations of (a) solid and (b) dissolved sodium chloride, (c) evaluate the relative strength of interactions present before and after the solvation process, and (d) represent the energy transfer required for the solution to form.

The second section considered the solvation process from a thermodynamic point of view. Students were reminded that the temperature decreased when sodium chloride dissolved, asked to predict whether changes in enthalpy, Gibbs free energy, and entropy would be greater than, less than, or equal to zero, and provide reasoning for their response. The final prompt in the activity asked students to "Explain why NaCl dissolves in water even though [the] process requires energy input from the surroundings”. For more details, see Appendix A for the complete activity as completed by students.

Similar representation items were also implemented on the applicable midterm exam in Spring 2014. These items served as summative assessment tasks to evaluate students’ ability to draw molecular-level pictures of both undissolved and dissolved ionic salts as seen below in Figure 4.4.

(a)

(b)



At the atomic-molecular level, **draw** what you think the $MgCl_2$ and H_2O samples look like **before** mixing:

At the atomic-molecular level, **draw** what you think the $MgCl_2$ and H_2O look like after mixing:

Figure 4.4 — Drawing prompts in summative assessment designed to elicit representations of (a) an undissolved ionic salt and (b) an aqueous solution of an ionic salt at the atomic-molecular level

The summative assessment items designed to elicit students’ representations of undissolved ionic salts (Figure 4.4a) and dissolved ionic salts (Figure 4.4b) are nearly identical in structure to the formative assessment items designed to elicit representations of undissolved ionic salts (Figure 4.3a) and aqueous solutions (Figure 4.3b).

Basis for revision

Initial analysis of student responses suggested that many students could successfully represent aqueous sodium chloride as being composed of sodium and chloride ions individually interacting with water molecules (the task from Figure 4.3b above). However, responses to the prompt shown in Figure 4.3d indicated that students were less successful at representing the atomic-molecular level collisions that must occur for energy to be transferred between the solvent and the intact solute.

Semi-Structured Interviews

A series of interviews was conducted at the end of the Spring 2014 semester to investigate how students connect their understanding of macroscopic energy changes to changes at the atomic-molecular level. These interviews were also intended to identify ways to improve instructional materials and assessments to better target students' prior knowledge and more successfully scaffold understanding across scalar levels from the atomic-molecular to the macroscopic observable for a range of topics explicitly connected to macroscopic energy changes in the CLUE curriculum.

Student participants were solicited for the study via email and pre-lecture announcements. Participating students were compensated two extra credit points toward the iClicker (attendance and participation) portion of their course grade. To provide further context on compensation, the CLUE section of GC2 apportioned 5% of the course grade to iClicker scores. There were 23 iClicker points available throughout the semester. Students were not permitted to earn more than full credit as a result of their participation in this research. Interviews were conducted at the end of the Spring 2014 semester after all relevant material had been covered in lecture, but before the course final exam. All students were informed of their rights as study participants and provided informed consent prior to participation. All participation was anonymous and confidential with respect to students' course instructors and teaching assistants. Pseudonyms are used throughout the interview findings to protect the privacy of participants.

<u>Protocol and rationale</u>

Interview tasks were designed to be similar to items students had previously encountered in both formative and summative assessments. This allowed for easier application of interview findings to the previously stated objective of improving curricular materials and assessments. Three contexts, resulting in four different phenomena, were selected to elicit students' explanations of macroscopic energy changes resulting from physical and chemical processes:

- Heating a pure substance
    - Heating and phase change of water
    - Comparison of heat capacities of ethanol and water
- Mixing of substances – solution formation
- Simple chemical reactions – combustion of methane

Of the four contexts, only the solution formation context is analyzed in this dissertation. This context prompted students to explain why a temperature increase was observed when potassium chloride dissolved in water. The interview protocol, including anticipated follow-up questions and prompts for further explanation, for this portion of the interviews is shown in Figure 4.5. The full interview protocol, including student materials and interviewer follow-up questions is included in Appendix B.

> In a beaker, you mix 500 mL of water and 50 g of KCl, a white solid.
>
> You observe that the white solid dissolves and that the temperature increases.
>
> Explain these observations.
>
> Follow-up questions and prompts for further explanation:
> - Explain why you think the temperature increases upon mixing.
> - What does the term exothermic reaction mean to you? Why would heat be released?
> - What happens at the molecular level?
> - Draw a molecular level picture: before and after dissolving the KCl?
> - If system/surroundings mentioned – describe what you mean by system and surroundings here?
> - If "stored" energy – why do you say energy is stored.
>   - How does the observed temperature change relate to changes in kinetic and potential energy as the species interact?

Figure 4.5 — Interview protocol and follow-up questions for solution formation context of semi-structured interview

The interview protocol was piloted with a graduate student to ensure clarity of prompts. For the full study, 22 students from CLUE chemistry courses volunteered. As shown in Figure 4.5, interview questions solicited students' ideas about the behavior, interactions, energy changes, and connections between atomic-molecular and macroscopic energy. The semi-structured interview format allowed the interviewer to ask follow-up questions to clarify student responses and attempt to elicit the entirety of each student's understanding. Preliminary analysis of the original formative assessment activity and the pilot interview resulted in a small number of pre-determined prompts which are referred to as "follow-up questions" and "prompts for further explanation" in the interview protocols in Figure 4.5 and Appendix B.

Interviews took approximately 45 minutes to complete. Audio and written work was digitally recorded with a Livescribe pen (http://www.livescribe.com/en-us/), which allowed audio to be linked with written work for future analysis. All student work was collected after each interview. After all interviews had been conducted, audio was transcribed by a commercial transcription service (http://accentance.com) and transcripts were compared to audio to ensure accuracy.

Analysis and findings

Interview data were analyzed inductively utilizing procedures influenced by open coding and constant comparison approaches to develop common themes present in students' responses (Corbin & Strauss, 2008). Because interviews were used primarily to provide direction and rationale for formative assessment activity revision, analysis focused on developing themes related to general successes, difficulties, and strategies for success encountered by students. We note that while the themes that emerged from these interviews are similar to what has already been discussed in the literature, they provided important verification of the ways students in the CLUE curriculum think about and explain ideas related to solutions and solution formation.

Common successes.

Many students were able to correctly identify the flow of energy required for breaking or forming attractive interactions. This is particularly important because of the many documented literature reports of students' difficulties with the endothermic nature of bond breaking (Boo, 1998; Teichert & Stacy, 2002) including very recent literature related to solutions and solution formation (Abell & Bretz, 2018; Bain & Towns, 2018). In Marissa's excerpt below, she is trying to explain why the temperature increased when potassium chloride dissolved.

Marissa:	[the temperature is] increasing because um, the energy between KCl, the energy put in, um to break the bond, is less than, the energy taken out when you form the bond.
Interviewer:	With that one you're thinking of, why does it take energy to break a bond? Like the bond between KCl?
Marissa:	why?
Interviewer:	yeah
Marissa:	because, there are attractions between the two atoms.
Interviewer:	mmhm
Marissa:	so, in order to overcome those attractions you have to put temperature or energy into it. To break it.

In her explanation, Marissa begins by stating that energy has to be added to break a bond. When the interviewer asks her why that might me true, she additionally notes that the bond is an attraction between potassium and chloride ions, and reiterates that you have to add energy to an attractive interaction to break it.

Students also were frequently successful realizing and using the idea that forming interactions requires that energy be released. Angelica started her explanation by stating that energy is released when new bonds formed. Over the course of her explanation she also talked about the structure of potassium and chloride ions, what new bonds might look like, and what it meant for the temperature to increase (in terms of more energy being released than absorbed) before the interviewer asked her to say more about the idea that forming interactions releases energy.

> Angelica: Energy was released when the new bonds between like water and potassium chloride were formed.
>
> [later]
>
> Interviewer: Now you mentioned that you thought the temperature change would be related to the amount of heat energy it takes to break the bonds as opposed to released when bonds are formed. Why do you think it is that energy would be released when a bond is formed?
>
> Angelica: Because (pause) I mean, when you have (pause) when you're breaking a bond, you have like two molecules that are like strongly attracted to each other so an outside force has to come in and like, break them. But when you're taking two molecules and you form them together, you're taking like both their energies and like combining them so it like releases energy.

Angelica was consistent in her reasoning that forming interactions releases energy. Furthermore, it appears that she was able to reassure herself by making an analogy to breaking interactions requiring energy when she was asked again to explain why forming interactions released energy. Her explanation of the process: "you're taking … both their energies and … combining them so it … releases energy" correctly implies that forming interactions lowers the potential energy of a system, requiring that energy be released.

The sophisticated understanding of energy and interactions used by both Marissa and Angelica is encouraging. Both of them were able to explain the energy required to change interactions by using reasoning based on attractive interactions rather than merely recalling the facts that overcoming interactions requires energy and forming interactions releases energy.

Common difficulties.

A range of difficulties was observed in students' responses to the solvation formation context that made it more difficult for them to successfully explain the increase in temperature.

Students often only considered the consequences of breaking *or* forming interactions, not the balance of the two. In the example below, Margaery answers a question about why the temperature would increase by referring to energy being released when bonds are broken.

Interviewer: So let's say that you have a sample of water and a sample of KCl, and you mix the two of them together and you observe that the temperature increases. Why do you think the temperature would increase upon mixing? How could you explain that?

Margaery: Probably because in the chemical reaction, there would be a breaking of bonds releasing energy. So if you drew it out, I guess, (DRAWING) it would turn (pause) it would become hydrochloric acid and potassium hydroxide. Yeah. And because of the breaking … of bonds it would release energy.

[later]

Interviewer: Now this idea of stored energy; just so that I'm thinking about it the same way that you're kind of thinking about it. What causes energy to be stored in a chemical system, let's say?

Margaery: I believe the energy is stored in the bonds between two different elements.

Later Margaery repeats this idea and elaborates that the energy that was released is stored in the bonds between elements. While it is true that potential energy is stored in fields, the idea that energy is stored in bonds is potentially problematic because it implies that energy can be obtained from bonds simply by breaking them.

Similarly, some students tried to use the idea that forming interactions required energy. In this excerpt, Maliah initially only compares the magnitude of the change in energy that occurs when new interactions are formed to what happens when bonds are broken. When asked specifically whether forming a bond releases or requires energy she then states that energy is required to form a bond.

Interviewer: Okay. And when you form those new interactions, is there any change in energy there?

Maliah: Yes, but it's smaller than the change in energy when the bonds are released.

Interviewer: Okay, so when you form a bond, is that releasing energy or taking energy?

Maliah: Well, actually it takes energy to form a bond

Another common difficulty observed in student responses was more subtle than examples of breaking bonds releasing energy or forming bonds requiring energy.

Chloe: Temperature increases in a substance when it's exothermic. Because energy's being released to its surroundings, so that means that there are bonds forming. And these bonds that are forming are going to be the ones that are when the water molecules go and attach themselves, like the hydrogen attaches itself to chloride and the oxygen's hanging out with potassium. And because of the formations, the formations are what's going to give us these temperature increases, as well as when we add a substance, an ionic substance like potassium chloride to water

In Chloe's response, she only considers the transformation that "agrees" with the temperature change observed for the overall process. While the statement "energy's being released to its surroundings, so that means that there are bonds forming" is certainly correct, it does not capture all of the components of the solvation process. It is important that students understand that observable temperature changes result from the sum of all energy requiring and releasing processes of a phenomena. If the temperature change is understood as the balance of these energy flows, it follows that all solvation processes are similar (in that they are composed both of steps that release and require energy). The alternative would mean that dissolving substances with negative enthalpies of solvation would proceed by a different mechanism than the dissolving of a substance with a positive enthalpy of solvation.

Student strategies for success.

Strategies for success are things that students said that helped them reground themselves and proceed to successfully explain the phenomenon. These are sort of “touchstones” to refocus their thinking, or reorient them in a direction that they remember being fruitful.

In the example below, Kent appears to get confused by how to account for the apparent temperature of the solution. He references the plastic bags of calcium chloride in water that were passed around during lecture to illustrate an exothermic solvation process. However, he is able to recall that the system that must be either absorbing or releasing energy is actually the individual dissolved ions and their respective hydration shells.

Interviewer: You mix them together and observe that the white solid dissolves and that the temperature increases. So how could you explain that observation that the temperature of the solution increases?

Kent: This is something that really confused me when we first learned it because — how do I put it? I would think, like, well, if the temperature increases, that must mean that it’s exothermic, right? Because-, but the reaction is actually endothermic. Wait, hang on, I'm getting confused here.

[Later]

I was always really confused by that because I’m, like, I remember being passed around the little baggies with the white powder and the water in it. And I could feel that it was hot and so, I’m like, okay, so this is obviously really, really warm. There’s a lot of energy here, but where did this energy come from? If it’s exothermic and giving off heat, how come I feel this heat? So there must be some sort of energy input to make that water hot. But then I talked to [The Professor]

> about it and she's, like, "you don't think of the system as the whole thing. The system is the KCl powder, the hydration shell around it." And then the surrounding water is the surroundings. Not like my hand is the surroundings and what's going on in the bag is the system because then it wouldn't make any sense. So yeah, that was something that was confusing. So what is happening here is as the temperature increases? I guess that means that the bonds in the product in the solution are greater than the bonds in just the regular KCl. So what's happening is the water is breaking apart and dissolving this KCl and then it's forming these hydration shells around it. And the interactions with the KCl and the water are stronger. And so, when the bond is formed that, of course, releases energy. So the reason that the heat of the surrounding water is increasing is because this system right here is giving off energy because the new stronger interactions are being formed and that gives off energy

After remembering to focus on the system of hydrated ions that must be releasing the energy for the temperature to increase, Kent was able to successfully describe the interactions that were formed and recognize that the new interactions were stronger than those in the undissolved potassium chloride.

Formative assessment activity revision

<u>Strategy</u>

Findings from semi-structured interviews and preliminary analysis of the original formative assessment activity provided a strategy for revision to support student performance in representing the process of solvation and explaining observable temperature changes. Based on interview findings, there were three main objectives of activity revision: (*i*) maintain the successes observed in interview responses, (*ii*) provide scaffolding to increase the likelihood that students avoid common difficulties; and (*iii*) provide students' with opportunities to exploit strategies for success.

Additionally, preliminary analysis of the original formative assessment activity indicated that the primary difficulty in the existing activity was related to the prompt combining atomic-molecular representations with concepts of transfer of energy, system and surroundings, and overall energy changes resulting in an observable temperature change. Therefore revision also focused on separating many of these ideas to help students think about them sequentially and deliberately before constructing a more coherent understanding.

Because the current research focuses on students' ability to (*i*) represent the solvation process at the atomic-molecular level and (*ii*) explain why a given observable temperature change might accompany the solvation process, only modifications to these aspects of the formative assessment activity will be discussed in detail. Modifications to portions of the activity dealing with enthalpy, entropy, and Gibbs free energy changes will be mentioned, but are not the focus of this research.

There were two main versions of the revised formative assessment activity, the first was first administered in Fall 2015. This version will be the primary focus of the following discussion of assessment revision. A final revision was completed and first administered in Fall 2016. Relevant changes made to produce this final formative assessment activity will then be discussed. For reference, the original formative assessment activity designed prior to this research is given in its entirety in Appendix A.

<u>Assessment revision</u>

The revised formative assessment activity begins quite similarly to the original activity in that students are asked to draw sodium chloride as a solid and after it has dissolved in water. In the first revision shown below in Figure 4.6, these representations are then brought forward in the activity, students are asked to compare them, and are then explicitly directed to identify specific interactions that are overcome (Figure 4.6a) and formed (Figure 4.6b). Ideally students will have drawn undissolved sodium chloride as a lattice or grid of alternating sodium and chloride ions, and dissolved sodium chloride as individual sodium and chloride ions independently interacting with the partially negative oxygen in water (for sodium ions) or the partially positive hydrogens in water (for chloride anions). In these cases, it would be the ionic bonding interactions in the crystalline salt that were overcome, while ion-dipole interactions would be formed.

(a)

(b)

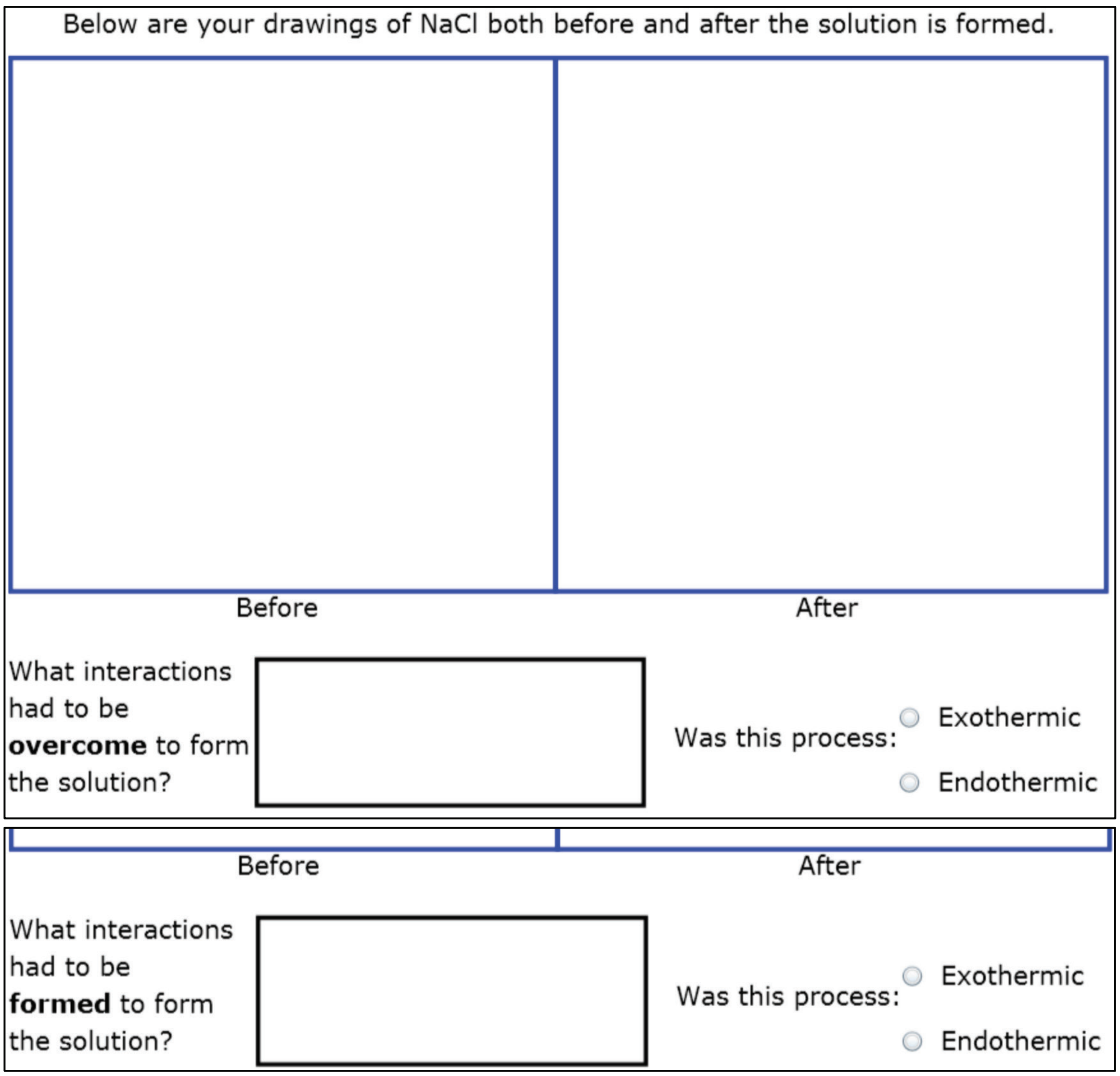


Figure 4.6 — Scaffolding implemented to assist students to make explicit the energy required or released as interactions are (a) overcome or (b) formed

The prompts shown above in Figure 4.6 address the revision strategy in two ways. First, initial student successes in correctly identifying the energy required to overcome or form interactions are reinforced by explicitly asking students whether overcoming and forming interactions are endothermic or exothermic. Second, the pair of tasks here, explicitly asking students about *both* the interactions overcome *and* the interactions formed, is intended to help students avoid one of the observed difficulties: that reasoning about temperature change often only referenced the transformation that coincided with the overall energy flow. By calling special attention to both interactions breaking and forming it is hoped that students will begin to think about the *balance* of changes of interactions taking place during the solvation process.

After answering the same question about the relative strength of interactions as in the original activity (Figure 4.3c), students are prompted to "draw a molecular level representation of the sequence of events required for NaCl to dissolve". The response area of this slide has been constructed to explicitly prompt for representations of sodium chloride in (*i*) undissolved, (*ii*) dissolving, and (*iii*) dissolved states. It is our intention, since they will have recently drawn the undissolved and dissolved states, that students will be able to focus more on the dissolving pane and think about what has to happen with the ions, molecules, and interactions, in order for the aqueous solution to form. The ideal representation for the dissolving pane would include solvent molecules, an intact solute, and interactions (or perhaps collisions, although collisions will look quite similar to interactions in a static representation such as those produced by students in this task) between the solvent (water in this case) and that intact solute.

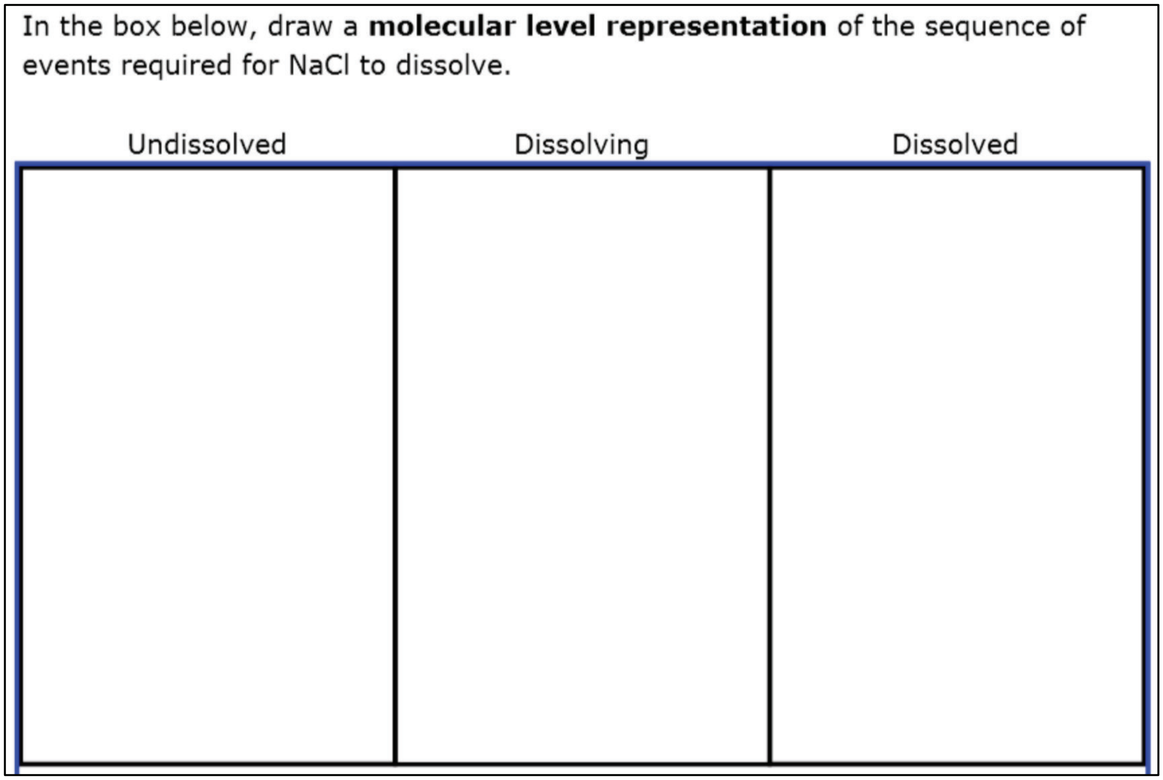


Figure 4.7 — New representation task prompting students to explicitly draw the mechanism by which sodium chloride ions are removed from each other, in addition to undissolved and dissolved states

The next three slides focus on the main strategy for success identified from interview data: the identification of system and surroundings for the solvation process. In the first of these slides, seen below in Figure 4.8a, students were shown their initial drawing of the dissolved aqueous solution of sodium chloride alongside a (potentially) more detailed cartoon of aqueous sodium chloride and asked to circle the system in the provided cartoon. The next slide allowed students to see what they previously selected for the system and compared it to one example of how the system could have been selected (see Figure 4.8b). Finally, in Figure 4.8c, students were asked to explain the importance of defining the system as the species that have formed new interactions as a result of the solvation process.

(a)

(b)

(c)

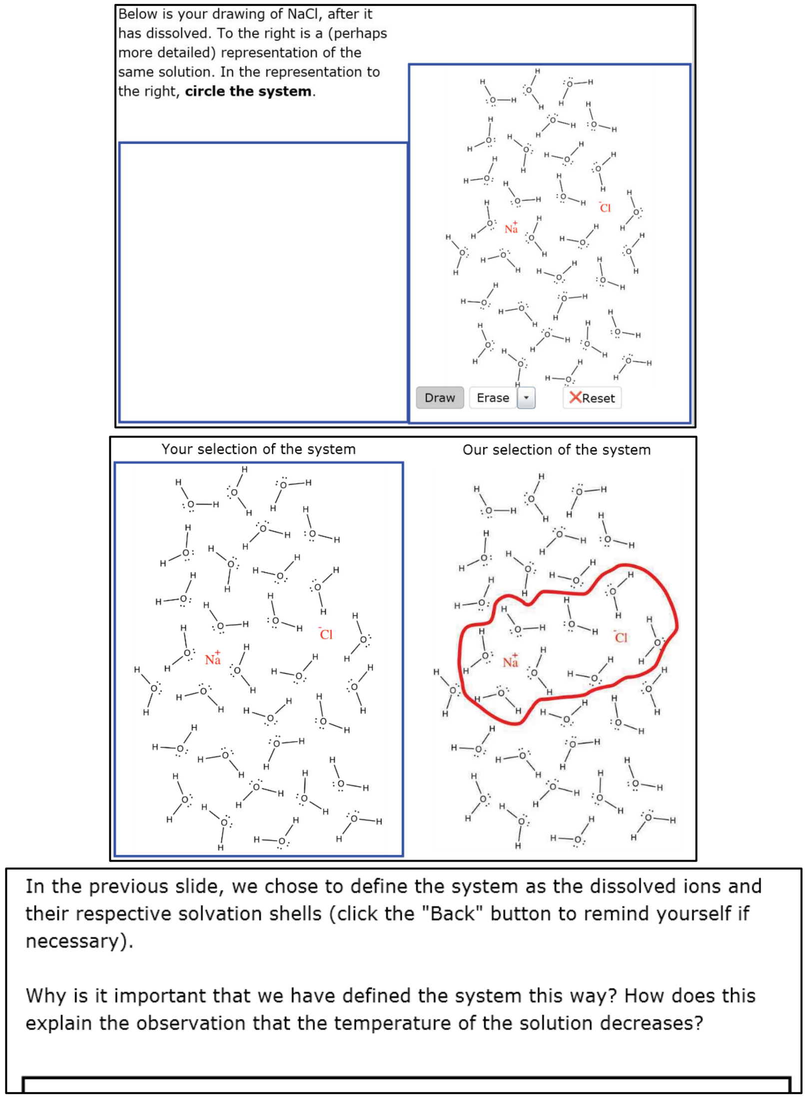


Figure 4.8 — Slides from revised formative assessment activity targeting student understanding of system and surroundings. Students were asked to (a) select the system, (b) compare their selection of the system to a provided representation of the system, and (c) explain the importance of defining the system appropriately

Following the slides related to the selection of system and surroundings, the original representation of the solvation process (as originally completed in Figure 4.7) is provided back to the student with instructions to change anything that needs to be changed to better show the process at the molecular level. It is important to note that throughout the formative assessment activity students are not allowed to navigate to previous tasks. Because students cannot work "backwards", they are given an opportunity to reevaluate and revise their initial representation of the solvation process. Because of the opportunity for revision, it is this second opportunity with the representation task that is most representative of student understanding of the solvation process by the end of the activity. By constructing the solvation representation task in this manner, it is our hope that providing students multiple chances to engage with the difficult task of representing the mechanism of solution formation, particularly with additional practice in the interim, will support student success and understanding. Furthermore, by providing explicit opportunities for students to engage with electrostatic and bonding interactions and how they must be overcome and formed for solvation to occur we hope to provide multiple ways and opportunities for students to organize their understanding.

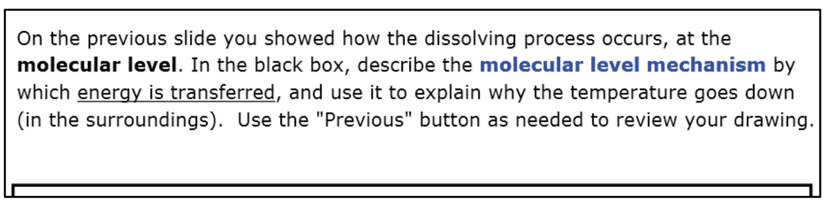


Figure 4.9 — Initial revised formative assessment activity explanation prompt for mechanism of energy transfer and observed temperature change

Following revision (as needed) of their representation of the solvation process, students were asked to describe the molecular level mechanism by which energy is transferred and explain why the temperature of the solution decreased as shown in Figure 4.9.

The final section of the revised formative assessment activity, which considered the solvation process from a thermodynamic point of view, was largely unchanged from the original activity. Changes to prompts related to the entropy change of the dissolving process are shown in Figure 4.10. The modifications to these questions were intended to provide more context (by including the equation for ΔG or providing a summary of the thermodynamic parameters of the solvation process) or suggest additional ways to think about the process itself (asking for an atomic-molecular level description of a change in entropy).

Original Formative Assessment Activity — Revised Formative Assessment Activity

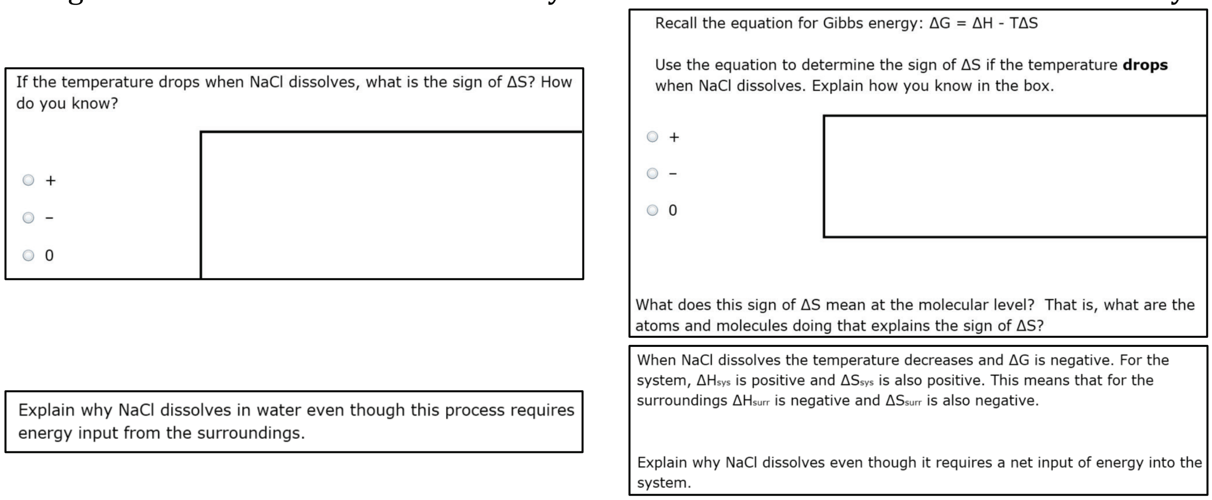


Figure 4.10 — Prompts from original and revised formative assessment activities related to the entropy change related to the solvation process

The last revision to be discussed in this section concerns the temperature change explanation prompt (originally shown in Figure 4.9 and reproduced below as Figure 4.11a). Initial analysis of this prompt (which will be further discussed in Chapter 6) showed that students had difficulty explaining why the temperature changed during solvation. The variety of responses also made analysis difficult because of the few common themes observed. Further consideration of the structure of the prompt indicated that the prompt itself was poorly worded and did not adequately signal what was actually important. Reading the initial revised prompt line-by-line, there are six things students have to consider and address to adequately respond: (1) the representation of the solution process the student just drew, (2) that this process occurred at the molecular level, (3) they need to describe a *different* mechanism that occurs at the molecular level, (4) this new mechanism will transfer energy, (5) the student then needs to explain a decrease in temperature, and finally, (6) that the previously drawn representation is available to look at again if the student needs to review anything. Finally the student must organize all of these components into a single coherent response in one large textbox.

The final revision cycle applied to the temperature change explanation prompt focused on supporting students in constructing an explanation by leveraging existing literature on the educative value of constructing and using explanations in science. Braaten and Windschitl (2011) constructed a tool to help middle and high school science teachers characterize and evaluate their students' explanations. This "Explanation Tool" identifies three types of explanations of increasing depth: *What*, *How*, and *Why*, that characterize explanations from purely descriptive and concerned with surface features (*What*) all the way up to full causal explanations leveraging unobservable or theoretical components to account for observable phenomena (*Why*). The intermediate *How* type describes explanations that incorporate components beyond surface features, potentially including some consideration of theoretical or other components of a smaller grain size that the phenomenon being explained. We note that the *Why* category of the Explanation Tool exhibits large overlap with the operationalized definition of mechanistic reasoning as necessarily including causal components of a grain size smaller that the phenomena being explained (Krist et al., 2018).

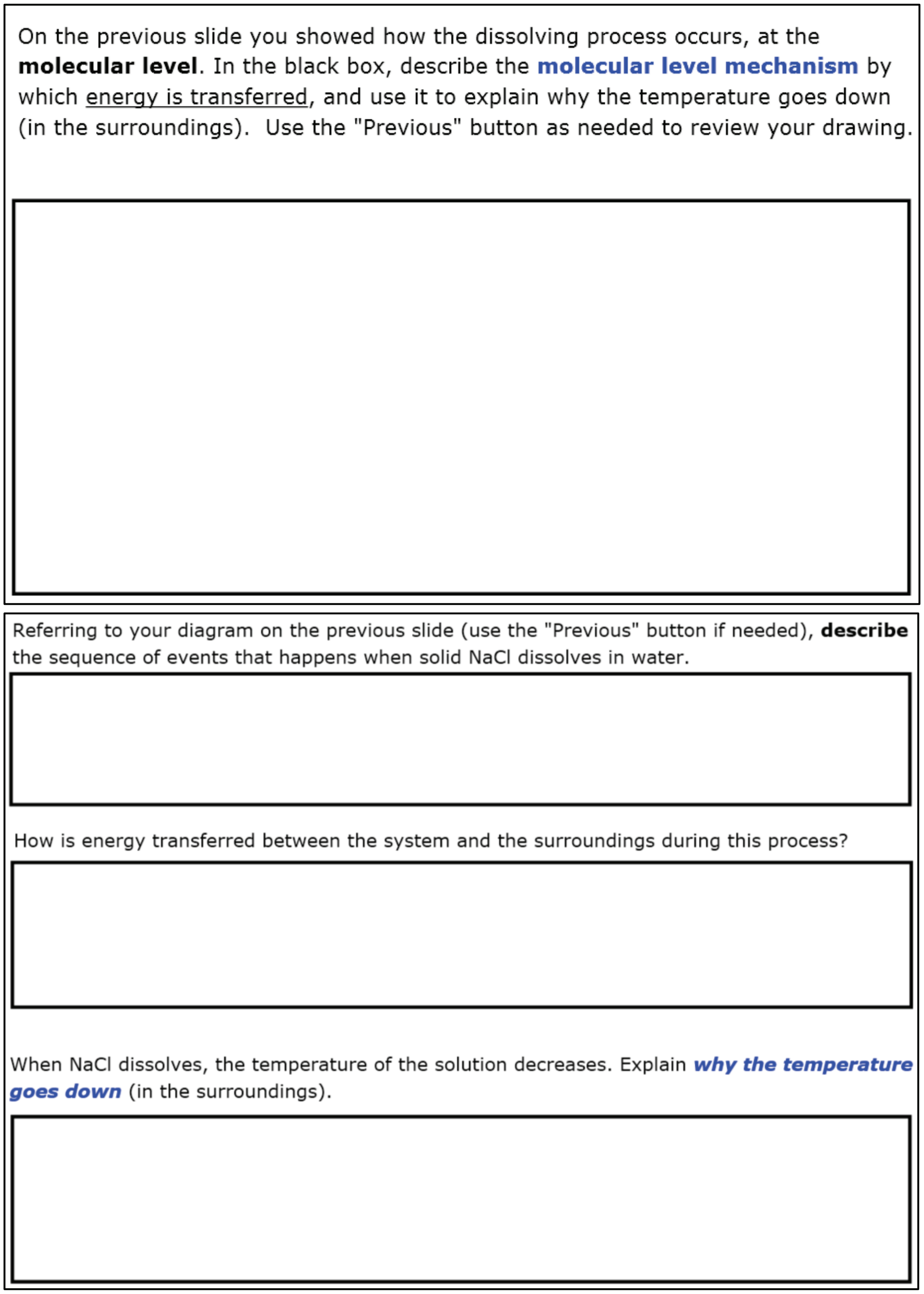


Figure 4.11 — First revised (a) and final revised version (b) of temperature change explanation prompt in the formative assessment activity

The Explanation Tool was used as a template of sorts to help students construct their explanation of the temperature change. The prompts on the final revised temperature change explanation prompt (shown above in Figure 4.11b) deliberately start with a *Why* level task (describe the sequence of events), with the intention that this more surface level request will be easier for students to productively address. The next prompt (how is energy transferred) is intended to elicit a *How* level response. Presumably, explanations of the energy transfer mechanism will include interactions or collisions between portions of the solvent and the solute, hopefully leading students to begin thinking “smaller” than molecules by considering what it is about the atomic structure of the solute and solvent that would promote the formation of new interactions.

In addition to gradually increasing the depth of explanation requested in successive prompts, the final revised task is intended to reduce the number of things students have to consider at any one time by splitting up the earlier task into three sections. By dividing the original prompt into multiple smaller tasks this final revised version is able to elicit specific responses in a defined sequence that has been designed to reveal how students understand the mechanism and energetic considerations of the solvation process. This structure also utilizes a scaffolding strategy that is intended to call students’ attention to components that they may have been taken for granted (Reiser, 2004) and prompt (explicitly in this case) students to explain and reflect of the phenomenon.

As stated previously, revision of the formative assessment activity was an iterative process. The first revised version, including the three-panel solvation process representation task (see Figure 4.7) and the single prompt temperature change explanation prompt (see Figure 4.11a), was introduced in the Spring 2015 semester. Fall 2015 was the first time students were able to review and revise their representations of the solvation process: the review and revise version of the representation task was added after the slides targeting system and surroundings. The last revision was implemented in Fall 2016, when the three prompt temperature change explanation task (see Figure 4.11b) was used. The final version of the formative assessment activity, as administered to students in the beSocratic system, is shown in full in Appendix C.

Assessment items

Two specific tasks from the revised formative assessment activity were chosen for further analysis. These are referred to as the Solutions Representation Assessment (SRA) and the Thermal Energy in Solvation Assessment (TESA). Both assessments are shown below, and are the basis for the rest of the research presented in this dissertation.

<u>Solvation Representation Assessment</u>

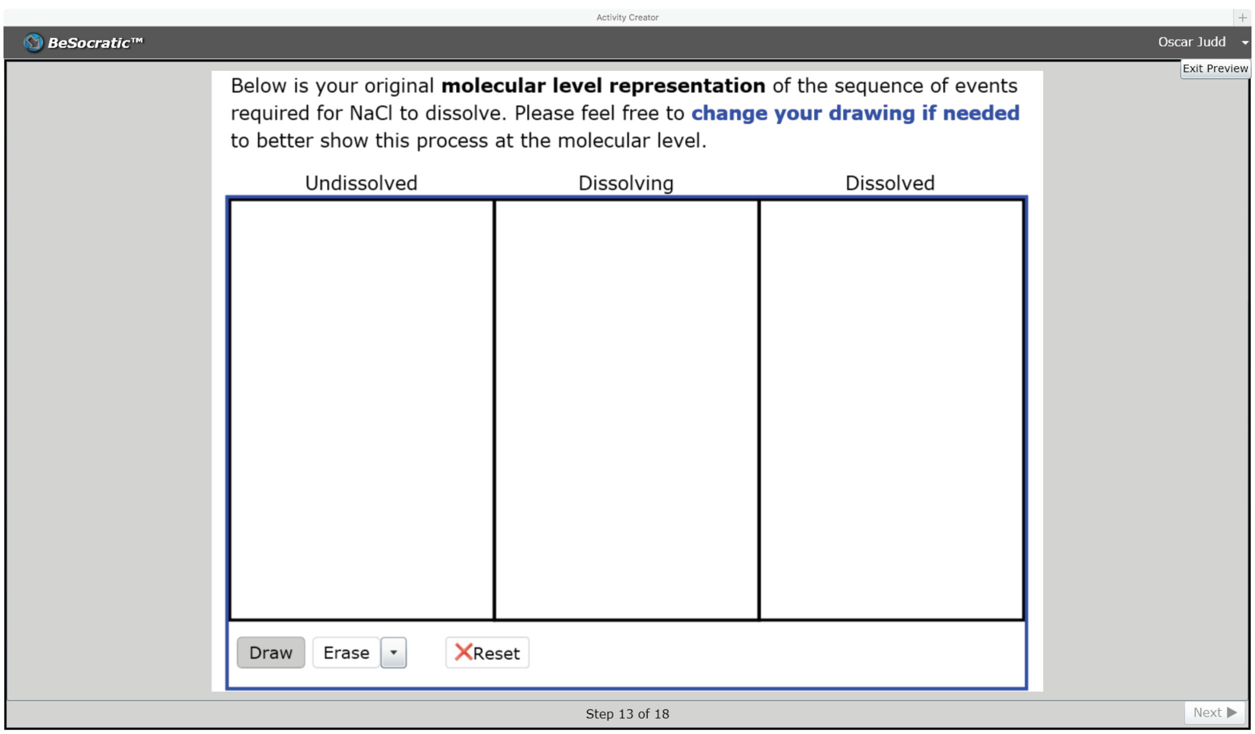


Figure 4.12 — Final version of the SRA, as seen by students completing the formative assessment activity, which was first implemented as a formative assessment task in Fall 2015

The three-panel representation task (referred to as the SRA) from the formative assessment activity was selected for analysis because it explicitly prompts students to show the solvation process at three “snapshots” in time: *before* the solute has begun to dissolve, as it is *dissolving*, and after it has completely *dissolved* and the aqueous solution is formed. By providing three different sections in the response area, this task is able to elicit the ways students visualize the solvation process in a way that allows researchers to confidently evaluate their representations.

As in the original solvation representation assessment task (formative and summative assessments shown above in Figure 4.3 and Figure 4.4, respectively), the SRA was adapted and implemented on the applicable midterm exam to evaluate students’ ability to draw molecular level pictures of the mechanistic process of solution formation in addition to undissolved and dissolved ionic salts. Sample items adapted for summative assessment are shown below in Figure 4.13. While the formative assessment version of the SRA does not contain a single three-panel response area, the three “snapshots” are explicitly included in single purpose prompts. That is, there is only a single instruction in each of the prompts designed to elicit each snapshot of the solvation process.

(a) (4 points) At the atomic-molecular level, **draw** what you think the separate KBr and H_2O samples look like **before** mixing, be sure to indicate such factors as relative numbers of particles and relative sizes :

(b) (6 points) At the atomic-molecular level, **draw** what you think the KBr and H_2O look like **as they are mixing, and explain in words what interactions are present**

(c) (6 points) At the atomic-molecular level, **draw** what you think the KBr and H_2O look like **after they are mixed, and explain in words what interactions are present in the solution.**

Figure 4.13 — Drawing SRA prompts adapted for summative assessment for (a) undissolved ionic salt (b) dissolving ionic salt, and (c) aqueous solution, at the atomic-molecular level

Thermal Energy in Solvation Assessment

The formative assessment prompts designed to elicit student explanation of the temperature change that occurs as a solution dissolves (referred to as the TESA) were selected for analysis because successful completion of this question *requires* that students relate a macroscopic observable phenomena (the change in temperature) to changes in interactions and energy at the atomic-molecular scale. This ability to link atomic-molecular scale behavior to macroscopic properties is central to chemistry, so student performance on this assessment is indicative of their ability to think and explain across scales while considering energy, structure and properties, and interactions. As mentioned above, there were two versions of the TESA administered in formative assessments, as shown below in Figure 4.14.

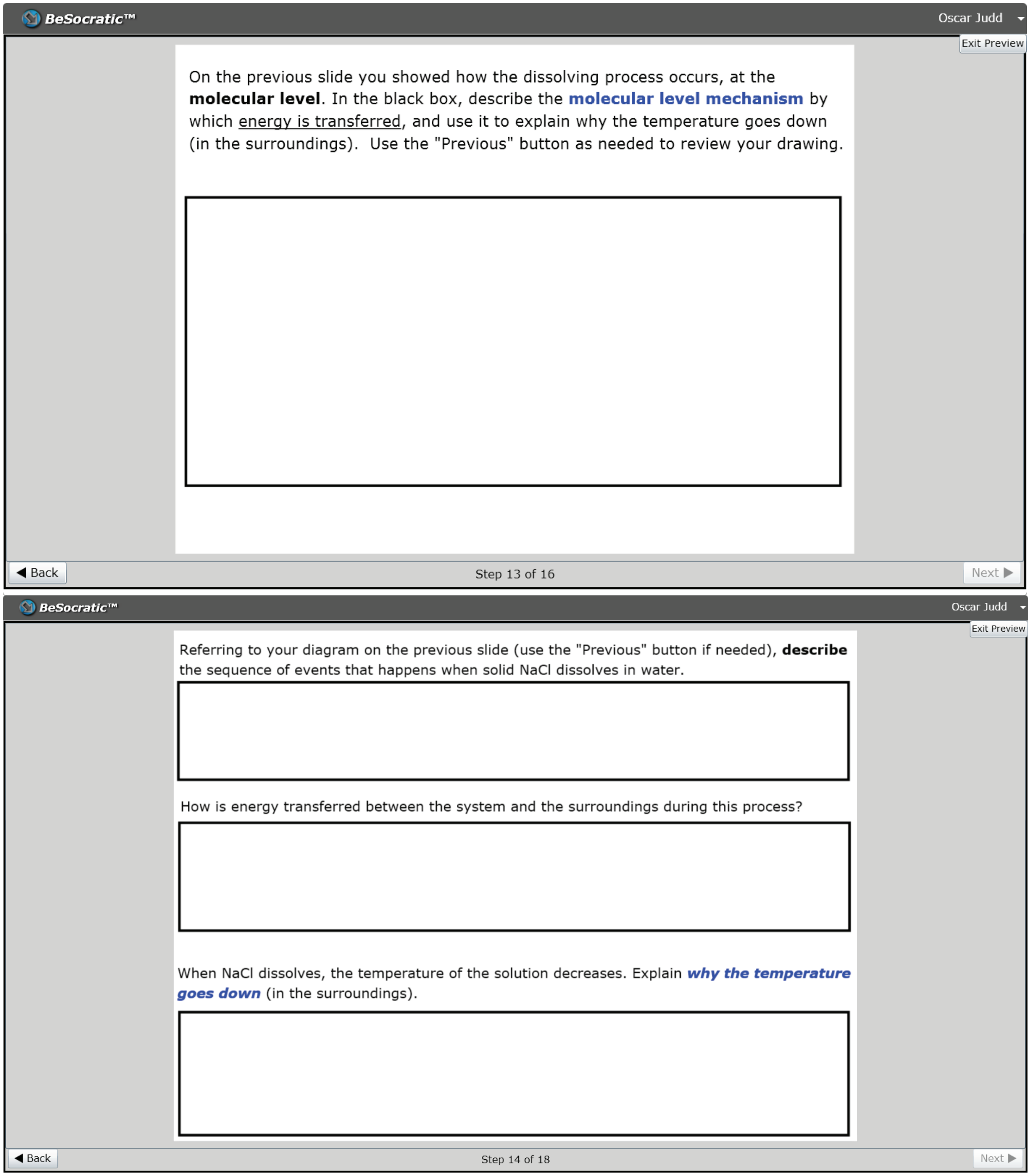


Figure 4.14 — First revised (top) and final revised (bottom) versions of the TESA, as seen by students completing the formative assessment activity, which was first implemented as a formative assessment task in Fall 2015 (top) and Fall 2016 (bottom)

As was the case with the SRA, the TESA has been modified for use in summative assessments to evaluate students' ability to explain a macroscopic observable phenomena using changes in energy and interactions occurring at the atomic-molecular level. An example of a summative assessment adaptation of the TESA is shown below in Figure 4.15. While the versions of the TESA used in summative assessment contexts do not include the prompt to describe the solvation process, the remaining prompts (explain the energy transfer mechanism and explain the temperature change) provide sufficient separation of instructions to support students to productively respond to these tasks.

(a) Now use your picture to explain the **mechanism** (process) by which energy is transferred at the molecular level during the mixing process.

(b) Using these interactions now **explain why** the temperature increases upon mixing $MgCl_2$ and H_2O.

Figure 4.15 — Explanation TESA prompts adapted for summative assessment for (a) explaining the mechanism of energy transfer and (b) explaining why the temperature changes during the solvation process

CHAPTER 5 — HOW DO STUDENTS REPRESENT SOLUTIONS AND SOLVATION?

In this chapter, I investigate student understanding of the mechanisms by which ionic substances dissolve in water. One approach to understanding how students conceptualize the process of dissolution is to have them construct representations that can be used to explain how and why the phenomenon occurs. Drawing can provide insights into the kinds of resources that students are using to construct explanations: it can make student thinking visible. By characterizing the kinds of representations of molecular level entities that students call upon, and by identifying the ways that these entities interact and change, we can begin to understand how a student conceptualized the solution process.

The research questions that guided this study were:

1. How do students represent solutions of ionic salts?
2. How do students represent the mechanism of the solution process?
3. What aspects of the task prompt are effective at eliciting evidence of student understanding?
4. How does the context of the task prompt (formative vs. summative) affect student responses?

Methods

Student participants

Student participants were selected from a population of second semester general chemistry students enrolled in the CLUE curriculum from Spring 2014, Fall 2015, and Spring 2016 semesters. As the second of a two-semester course sequence, second semester general chemistry (GC2) has an average spring ("on sequence") enrollment of 800 students and an average fall ("off sequence") enrollment of 400 students. From these populations, cohorts of 75, 100, and 100 students were randomly selected from Spring 2014, Fall 2015, and Spring 2016 semesters, respectively. Demographics of each cohort are shown below in Table 5.1. The demographic data for each cohort are not statistically different from those of the populations from which they were selected.

Table 5.1 — Gender, class standing, ethnicity, and common majors for Spring 2014, Fall 2015, and Spring 2016 cohorts. Relevant p-values for Chi-square tests are included; significant differences are indicated in bold.

Demographics	Spring 2014 (N=75)	Fall 2015 (N=100)	Spring 2016 (N=100)	p-value
Gender	52% Female 48% Male	60% Female 40% Male	62% Female 38% Male	0.386
Class Standing	79% Freshman 16% Sophomore 5.3% Upperclass	16% Freshman 49% Sophomore 35% Upperclass	40% Freshman 30% Sophomore 30% Upperclass	**<0.001**
Ethnicity	77% White 9.3% Asian 13% URM	66% White 9.0% Asian 25% URM	63% White 8.0% Asian 29% URM	0.184
Common Majors	24% Premedical 16% Human Biology 7.9% Kinesiology	16% Human Biology 6.7% Premedical 6.0% Kinesiology	20% Human Biology 15% Premedical 4.7% Kinesiology	N/A

Each cohort is not statistically different from its respective total enrollment in terms of distribution of gender, class standing, or ethnicity. Additionally, all three cohorts are not statistically different from each other in terms of gender or ethnicity distribution. As indicated by the p-value of the relevant chi-square test (<0.001), the distribution of students' class standing is not statistically equivalent across the three cohorts.

The 2013-2014 academic year was the first implementation of the CLUE curriculum at a new university. The first course of the CLUE sequence was taught as one of six lecture sections of first semester general chemistry offered in Fall 2013; the second course was one of two lecture sections of second semester general chemistry offered in Spring 2014. Because the CLUE curriculum is designed as a two semester sequence, special care was taken to ensure that students were able to enroll in both semesters of the CLUE sequence if at all possible. By Spring 2015, all general chemistry courses at this university used the CLUE curriculum, making the Fall 2015 cohort the first time that second semester CLUE was taught "off-sequence". The final cohort in this study, Spring 2016, was the first time the final assessment (described in detail below) was administered to students in an "on-sequence" second semester CLUE course.

All students were informed of their rights as study participants and provided informed consent prior to participation. All participation was anonymous and confidential with respect to students' course instructors and teaching assistants.

Solvation Representation Assessment

The Solvation Representation Assessment (SRA) was used to elicit students' understanding of the process by which solvation occurs, and is shown below in Figure 5.1. The response area of the SRA has been constructed to explicitly prompt for representations of sodium chloride in (*i*) undissolved, (*ii*) dissolving, and (*iii*) dissolved states.

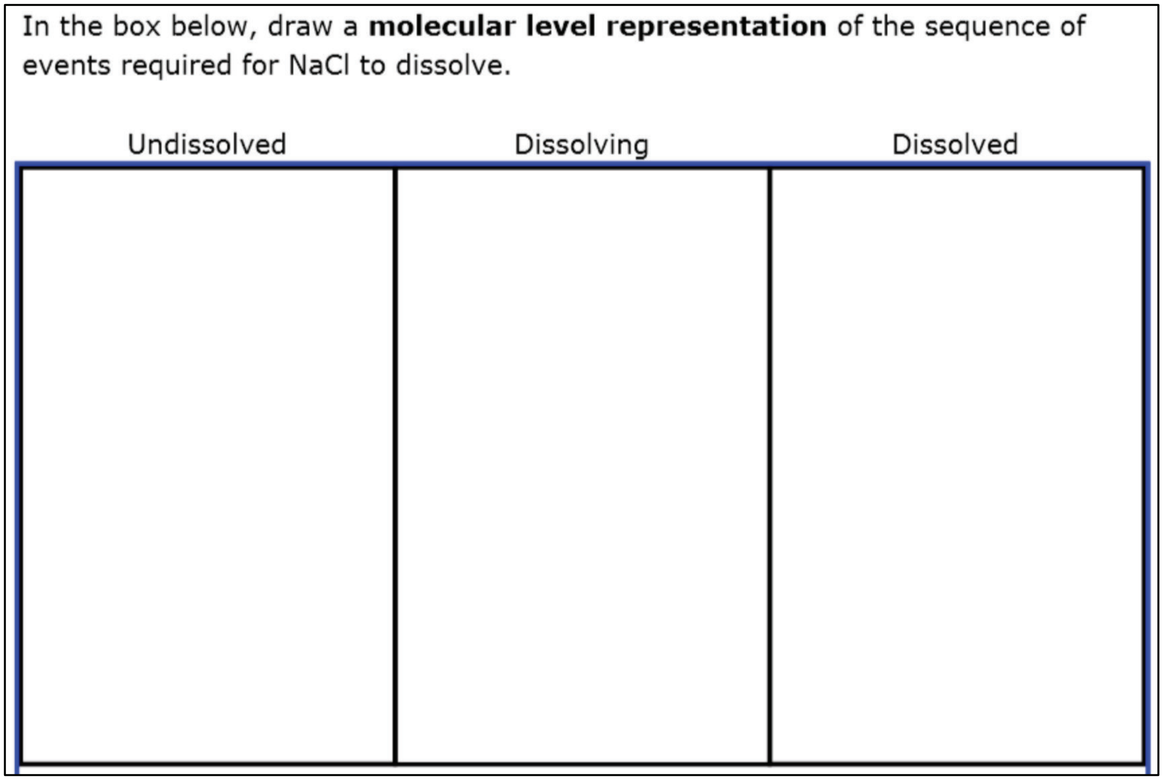


Figure 5.1 — SRA task prompting students to explicitly draw the mechanism by which sodium chloride ions are removed from each other, in addition to undissolved and dissolved states

An exemplar response to the SRA is shown in Figure 5.2. The ideal representation for the dissolving pane would include solvent molecules, an intact solute, and interactions between the solvent (water in this case) and that intact solute. The ideal representation for the dissolved pane would include isolated sodium cations and chloride anions, each individually interacting with the appropriate parts of the solvent molecules: the δ+ hydrogens will interact with the chloride anions while the δ– oxygens will interact with the sodium cations. There are also water molecules with hydrogen bonding interactions that are outside the hydrations spheres of the ions.

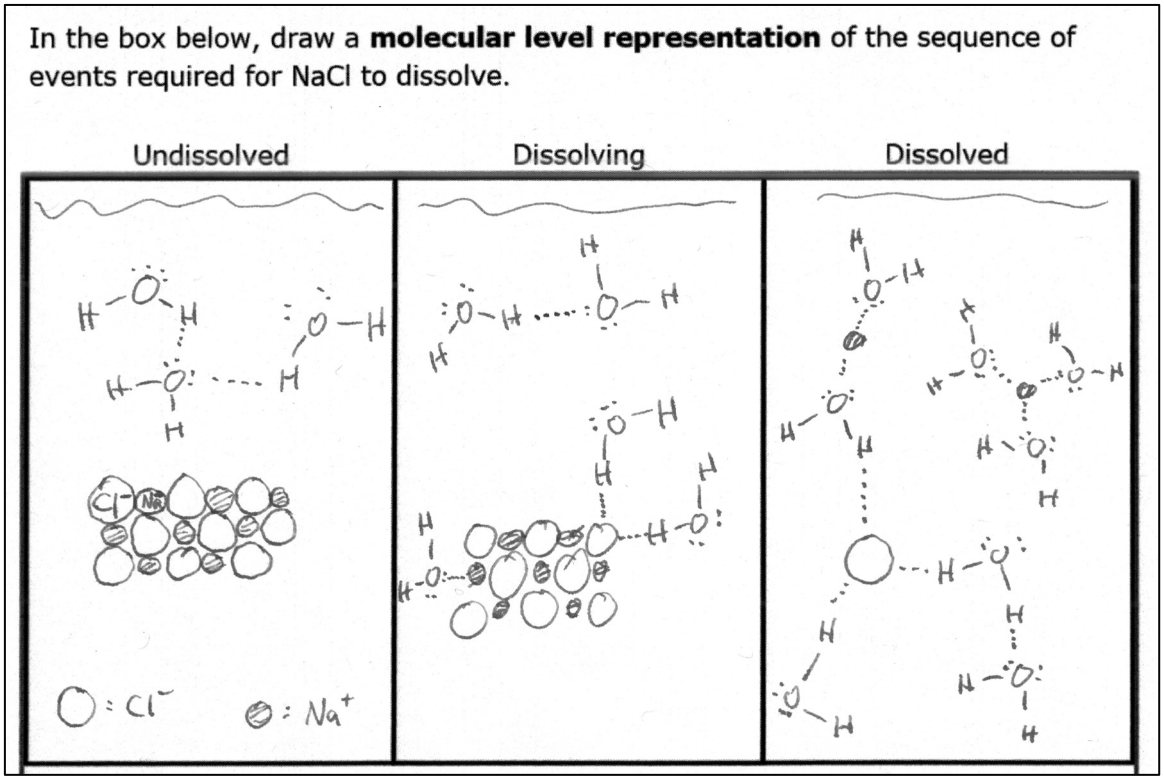


Figure 5.2 — Exemplar response to Solvation Representation Assessment

The SRA was adapted and implemented on the applicable midterm exam to evaluate students' ability to draw molecular-level pictures of the mechanistic process of solution formation in addition to undissolved and dissolved ionic salts. Sample items adapted for summative assessment are shown below in Figure 5.3.

(a) (4 points) At the atomic-molecular level, **draw** what you think the separate KBr and H_2O samples look like **before** mixing, be sure to indicate such factors as relative numbers of particles and relative sizes :

(b) (6 points) At the atomic-molecular level, **draw** what you think the KBr and H_2O look like **as they are mixing, and explain in words what interactions are present**

(c) (6 points) At the atomic-molecular level, **draw** what you think the KBr and H_2O look like **after they are mixed, and explain in words what interactions are present in the solution.**

Figure 5.3 — Drawing prompts adapted for pencil and paper summative assessment for (a) undissolved ionic salt (b) dissolving ionic salt, and (c) aqueous solution, at the atomic-molecular level

It is important to note that, while the SRA is completed as part of a larger homework activity for the formative assessment data presented below, students are not provided with a written answer key to homework tasks. This is true throughout the CLUE curriculum in general, and specifically for the SRA.

Analysis

Student responses were analyzed inductively in an iterative process utilizing procedures influenced by an open coding approach with constant comparison; initial coding also used some of the findings from student interviews to inform preliminary code categories (Corbin & Strauss, 2008). Generally, data were analyzed through three phases to develop the final coding scheme for the current research: initial coding, axial coding (to consolidate initial codes and start developing themes observed in student responses), and coding for interactions.

Developing the Coding Scheme

Initial analysis focused on surface level features of representations in order to document the breadth and frequency of different types of responses. These features were primarily descriptive, and examples of codes applied in this phase of analysis are shown in Table D.1 located in Appendix D. Primary groups of codes describing representations of the solution process included the scale of the representation drawn, if and where interactions were first explicitly used in the representation, and components included in the representation. Additional codes described if students reset the drawing tool while constructing their representation and whether their final representations were similar after resetting.

Further analysis sought to organize these initial codes into more generalizable classifications of the sorts of representations students produced as well as begin to develop codes to capture themes observed in the data. During this phase of analysis features specific to each of the “dissolving” and “dissolved” panes of the SRA were identified and existing codes were refined. Some new codes generated and applied in this process noted the presence of an intact solute in the “dissolving” pane, solvated ions in the “dissolved” pane, explicit addition of energy to the system, chemical reaction of the solute with water, and appearance of the solute as ionic “molecules”. Refined and new codes applied during this phase of analysis are summarized in Table D.2 located in Appendix D.

The codes presented in Table D.1 and Table D.2 in Appendix D describe features of student representations of the solution process and are not intended to holistically describe the extent to which the representations are canonically accurate. The presence of inaccurate features was not taken into account except in cases where those specific features were the explicit focus of the code. Indeed, the simple descriptive nature of the codes developed in these preliminary analysis phases means that multiple codes were often applied to each student representation.

For example, the “solvated ions” code applied to the dissolved pane only requires that isolated solute particles are interacting with a solvent molecule; in the case of the “reversed polarity of interactions” example shown below in Figure 5.4, the “solvated ions” code was also applied. Finally, because the interactions are indicated by the orientation and proximity of the species (rather than explicit lines, dashes, or other explicitly drawn representation of the interaction), the “implicit interactions” code would also be applied.

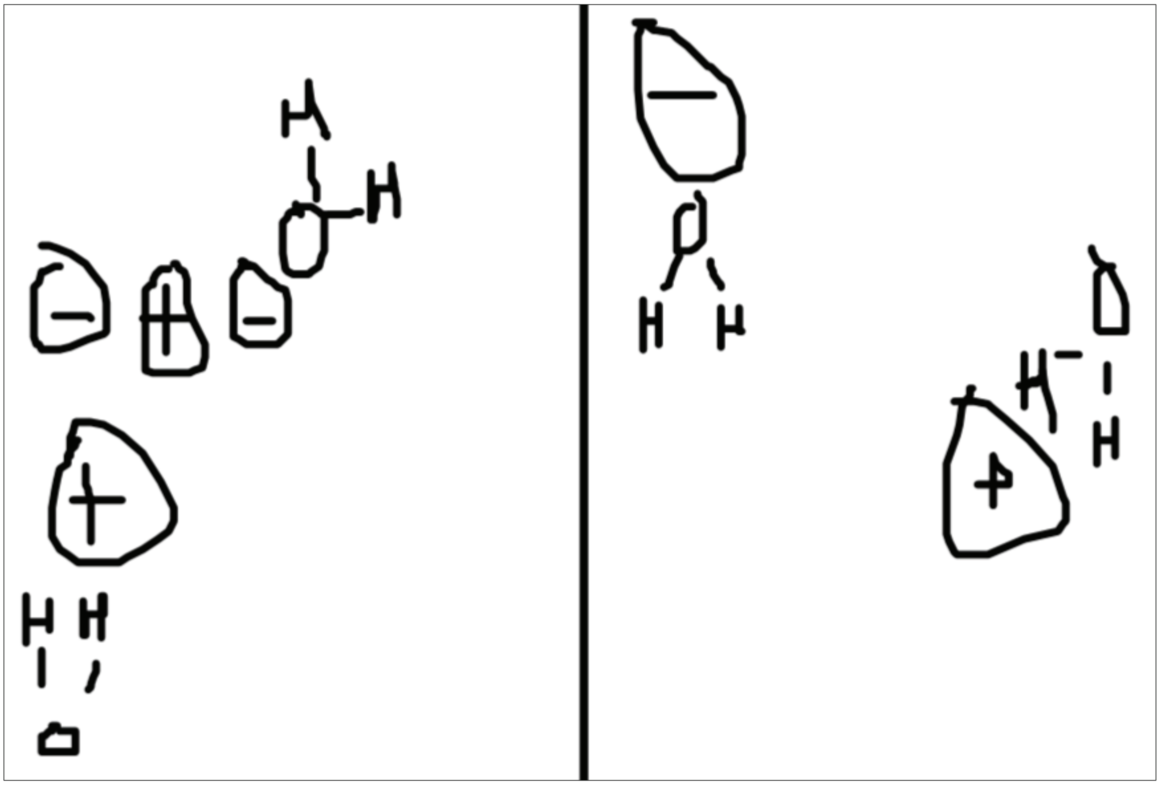


Figure 5.4 — Example of response containing "reversed polarity of interactions" in addition to "solvated ions" and "implicit interactions"

<u>Coding for Interactions</u>

While the previously discussed descriptive codes are useful for becoming familiar with the features that students include when representing the solution process, the large number of potentially co-occurring codes makes it difficult to develop an overall picture of the way representations were constructed by students. In fact, merely noting the many ways students can make mistakes or include incorrect features in their representations runs the risk of not capturing the ways students can be successful in performing tasks that the literature has shown to be very difficult.

With this in mind, final code development focused on generating a set of mutually exclusive codes to describe the range of representations observed. Due to the nature of the task, where students were instructed to draw a representation of the solution process at the atomic-molecular level, we chose to focus on students' use of electrostatic and bonding interactions. A set of mutually exclusive codes describing features of interactions in student representations was developed. Code examples and summaries are shown in Table 5.2 and further described below.

All of the codes were applied independently to the dissolving and dissolved panel of student representations and are mutually exclusive within the scope of each panel. For all codes, interactions can be either explicit (using dashed, dotted, or similar lines to indicate the presence of an attractive interaction between two species) or implicit (attractive interactions that are implied by proximity and orientation of two species and are systematically arranged in a consistent way). For more details, including additional exemplars and examples and explanation of edge cases, please see Appendix E for the complete codebook describing the coding scheme.

Table 5.2 — Summary of final codes as applied to student representations to describe students' use of interactions. Code exemplars are shown for both the "dissolving" and "dissolved" panels.

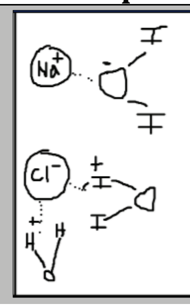
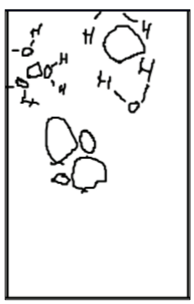
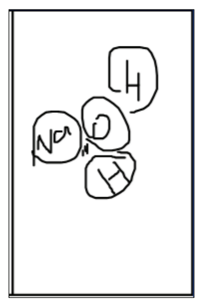
Code name	"Dissolving" code example	"Dissolved" code example	Code explanations
Complete Interactions (CI)			All structural and interaction components of representation are present, correct, and complete
Incomplete Interactions (II)			All structural components of representation are present and correct, but some interactions are not present. Commonly missing components: interaction between intact solute and solvent (dissolving) and not all solute ions interacting with solvent molecules (dissolved)

Table 5.2 (cont'd)

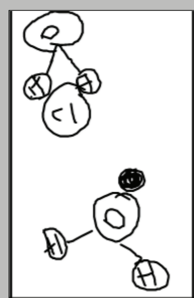
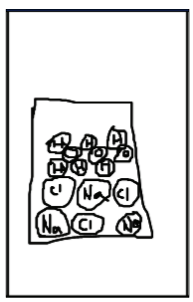
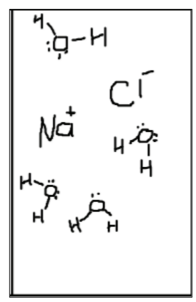
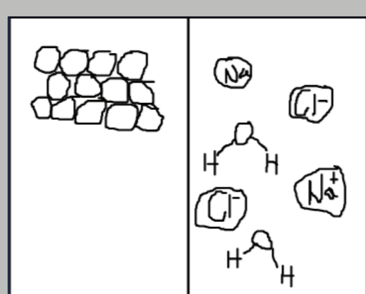
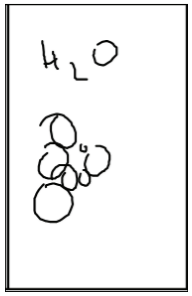
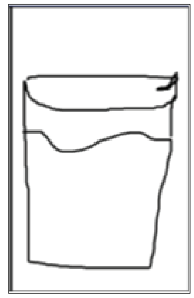
Code name	"Dissolving" code example	"Dissolved" code example	Code explanations
Some interactions, incorrect structure (SI)			Representation contains interactions (either explicit or implicit) between the solvent and the solute, but has incorrect structures, such as representations of ionic compounds as molecules
No solute-solvent interactions (NSSI)			Representations are at the atomic-molecular level, but do not contain interactions between the solvent and the solute
No Interactions (NI)			Particles that were present in the previous pane are no longer intact, ***and*** that there are no interactions present that would explain or account for how the previously associated ions or molecules became separated

Table 5.2 (cont'd)

Code name	"Dissolving" code example	"Dissolved" code example	Code explanations
Off Task (OT)			Representations that are not at the atomic-molecular level or otherwise uninterpretable

Complete Interactions

Representations coded as Complete Interactions (CI) are those with appropriate and complete interactions. For a representation in the "dissolving" panel to have complete interactions, there must be an intact solute present and there must be interactions between the solvent and that intact solute. There may additionally be solvated ions, although they are not required for the CI code to be applied. For a representation in the "dissolved" panel to have complete interactions, all ions must be interacting with the appropriate part of the solvent molecule (i.e. cations with δ– O, and anions with δ+ H) and there must be both cations and anions present and solvated in the representation. A single solvent molecule is sufficient for the ion to be classified as "solvated".

Incomplete Interactions

Representations coded as Incomplete Interactions (II) are those in which all included components are correct, but some components required for the Complete Interactions code are not present. For a representation in the "dissolving" panel to be given the II code all structural features of CI codes must be present, including an intact solute and solvent molecules, but the interactions between the solvent and the intact solute will be missing. It is the absence of these interactions between the solvent and the intact solute that makes such representations “incomplete” in our coding scheme. For a representation in the “dissolved” panel to be given the II code there will either be some solute ions not interacting with solvent molecules or only one ion type (cation or anion) will be included.

Some Interactions, Incorrect Structure

Representations coded as Some Interactions, Incorrect Structure (SI) are those with interactions present between solvent and solute that also contain an incorrect or incomplete structure. Features that are classified as incorrect structure include “covalent” representations of ionic compounds, lack of an intact solute (for “dissolving” pane), and ambiguous structures. As in previously defined codes, interactions must be present between solvent and solute for the SI code to be applied. However, there is no differentiation between “correct” and problematic representations of these interactions as this is the last code (least sophisticated treatment of interactions) that includes solute-solvent interactions.

No Solute-Solvent Interactions

Representations coded as No Solute-Solvent Interactions (NSSI) are those with appropriate (although not necessarily complete, as defined above) structures but no interactions between solute and solvent. Although complete structures are not required, representations in the “dissolving” panel must include solvent molecules and either an ionic lattice or isolated ions. Representations in the “dissolved” panel will include ions and solvent molecules, but no interactions between the ions and solvent. Often NSSI in the “dissolved” panel means that all components are present (except for the solute-solvent interactions), and that interactions were present in the “dissolving” pane that can explain the subsequent separation of the particles

No Interactions

The No Interactions (NI) code requires consideration of the preceding panel (i.e. "undissolved" when coding the "dissolving" panel or "dissolving" when coding the "dissolved" panel). Representations coded as NI are those where the solute has changed such that it is in smaller pieces, but without interactions in the preceding panel that can account for how the particles became separated; there are also no interactions in the panel to be coded.

Off Task

Representations coded as Off Task (OT) are those with either ambiguous structures and no interactions or representations that are not at the molecular level.

Once codes (summarized above in Table 5.2) were developed, reliability was evaluated by training an independent coder and comparing codes assigned to student responses. Through an iterative process, code definitions were applied and clarified as necessary; independent coding for the representations of solutions as solvated ions resulted in 87% agreement with a Cohen's kappa of 0.76 indicating substantial agreement (Landis & Koch, 1977). Representations of the dissolving process were more difficult to come to mutual agreement and therefore required further cycles of coding, code definition refinement, and analysis. Final coding resulting in 97% agreement with a Cohen's kappa of 0.95 indicating near perfect agreement (Landis & Koch, 1977).

Results and Discussion

<u>RQ1: How do students represent solutions of ionic salts after the dissolving process?</u>

Responses to the initial assessment (as seen in Figure 4.3b and Figure 4.4b) administered in Spring 2014 were coded to characterize student representation of aqueous solutions (that is, the final panel in the drawing task) using the same codes developed for the SRA. Results of coding the initial drawing task as administered in formative and summative assessments are shown below in Figure 5.5. From this data we can see that most students were able to successfully represent an aqueous solution of an ionic salt as being composed of separated ions interacting appropriately with molecules of the solvent in both tasks, as indicated by the large fraction of responses coded as CI. Nearly all responses (84%) were coded CI for the summative assessment task.

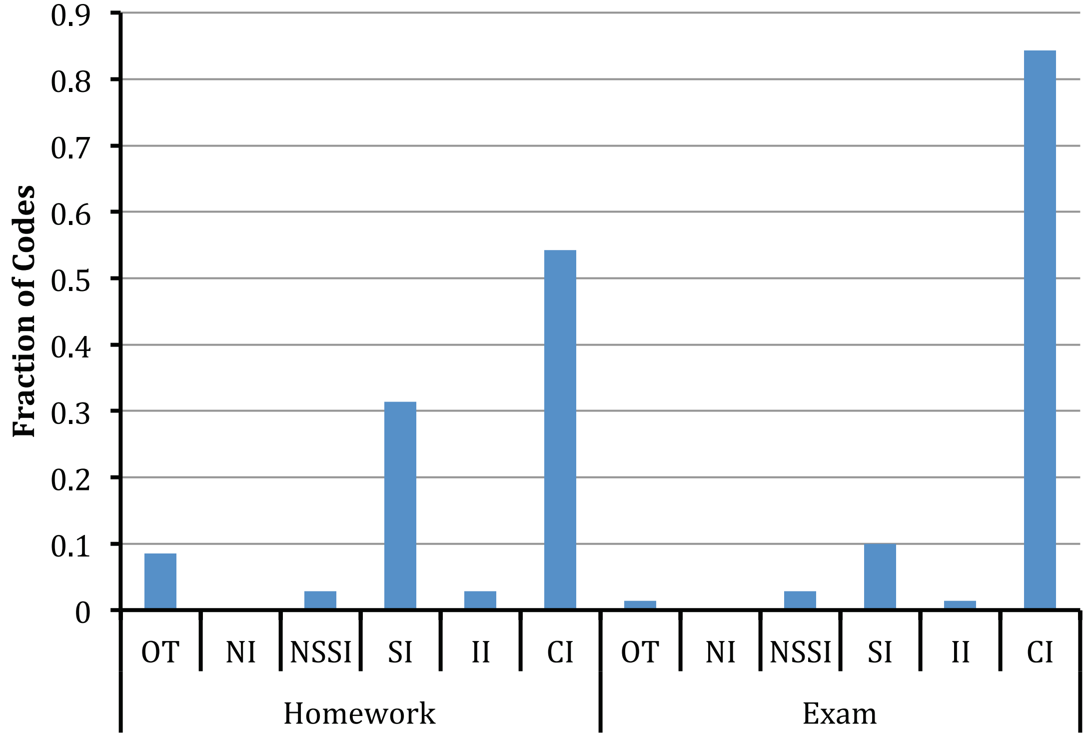


Figure 5.5 — Analysis of aqueous solution representation tasks from Spring 2014 as administered in formative and summative assessments. Code abbreviations along the *x*-axis are the same as previously defined in Table 5.2.

After assessment revision we wanted to ensure that changes made to the task did not impede students' ability to successfully represent aqueous solutions. Because the revised assessment requires students draw the fully dissolved solution multiple times, there was a possibility that student fatigue could result in less success representing solutions with correct interactions. Results for the two semesters immediately following implementation of the revised drawing prompt, Fall 2015 and Spring 2016, are shown below in Figure 5.6, represented by the red and green bars respectively; results from Spring 2014 are included for comparison and are represented by the blue bars.

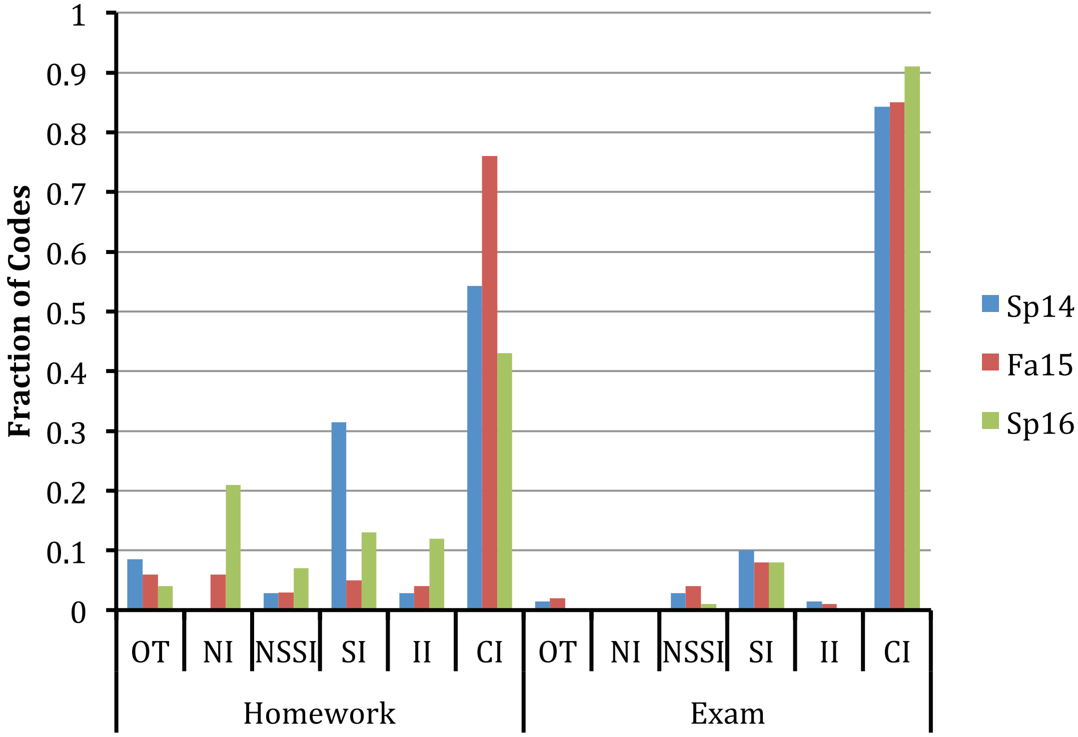


Figure 5.6 — Analysis of aqueous solution representation tasks from Spring 2014, Fall 2015, and Spring 2016 as administered in formative and summative assessments. Code abbreviations along the *x*-axis are the same as previously defined in Table 5.2.

The combined results show that overall most representations were coded CI for both homework and exam assessments. Furthermore, the largest non-CI groups in the homework assessment reduced from 31% in Spring 14 (the SI code) to approximately 5% and 13% for Fall 2015 and Spring 2016 cohorts, respectively. Results for exam assessments show that the vast majority of students' representations were coded as CI. The revision to include multiple drawing prompts did not decrease the incidence of CI codes.

Chi-square analysis was performed to further investigate how students from the different cohorts represented solvated ions; these results are shown below in Table 5.3.

Table 5.3 — Chi-square statistics comparing distribution of codes for representations of solvated ions in both homework and exam settings across cohorts. Significant differences are indicated by bold p-values

Assessment Type	Pearson Chi-Square	*df*	*p*-value	Cramer's V
Homework	60.719	10	**<0.001**	0.474
Exam	5.458	8	0.708	N/A

Results of the chi-square test ($\chi^2 = 60.719$, $df = 10$, $p < 0.001$) suggests we reject the null hypothesis that there is no association between semester and distribution of codes applied to formative assessment representations of solvated ions. Cramer's V provides a measure of association between nominal values; the value of 0.474 observed here indicates a medium to strong association (Cohen, 1988) between the distribution and the cohort. This was not unexpected due to the previously mentioned difference in cohort demographics (which were driven by differences in class standing; Fall 2015 had relatively more sophomores and relatively fewer freshmen).

While the distributions of codes from the formative assessment are not equivalent among the three cohorts, a majority of students were able to successfully depict isolated ions individually interacting with solvent molecules for all implementations (both homework and exam) of the solution representation task. In fact, despite the differences in cohorts (in both demographics and performance in representing solvated ions in homework assessments), results from coding summative assessment items show nearly all students (84%, 85%, and 91% for Spring 2014, Fall 2015, and Spring 2016 semesters, respectively) represented the aqueous solution with Complete Interactions. Chi-square analysis ($\chi^2 = 5.458$, $df = 8$, $p = 0.708$) indicates that the distribution of codes is not different among the three cohorts for representations of solvated ions in formative assessments. This is in stark contrast to extensive reports documenting the difficulties students have representing aqueous solutions as being composed of isolated ions each individually experiencing attractive interactions with solvent molecules (Abell & Bretz, 2018; Ebenezer, 2001; Herrington et al., 2017; Kelly & Jones, 2007, 2008; K. C. Smith & Nakhleh, 2011; K. J. Smith & Metz, 1996).

While it is certainly possible that students have memorized the diagrams of solvated ions, we attribute this success to the interconnected structure of the CLUE curriculum itself, and to the opportunity to practice the construction of models using beSocratic. Immediately preceding the formation of aqueous solutions of ionic salts were discussions of solutions of liquids (what liquids would or would not be soluble with each other); this analysis of the miscibility of liquids relies on students' ability to successfully negotiate the translation of molecular structure into molecular, and subsequently bulk material, properties (Cooper et al., 2012). It would appear that the structure of the CLUE curriculum (scaffolding of lecture, recitation, and homework activities) was successful in refining students' representations.

<u>RQ2: How do students represent the mechanism of the solution process?</u>

While most students were able to successfully represent solvated ions in solution, the situation is somewhat different for the process of solvation. We first analyzed the energy transfer representation task from the original formative assessment activity as seen above in Figure 4.3d to provide comparison against the more scaffolded SRA. Although the energy transfer representation task was not explicitly designed to elicit a representation of the solvation process itself, it *was* intended to prompt students to represent collisions between the solvent and the intact solute providing sufficient energy to overcome the attractive ionic bonding interactions holding the solute together. A representation of a collision between these species would also necessarily represent an interaction between the solute and solvent because of their proximity. Because such a representation would feature solvent molecules interacting with an intact solute and as such could reasonably be coded as having Complete Interactions, we analyzed these representations to see how students responded to the original mulitcomponent assessment prompt. The results of this analysis are shown below in Figure 5.7, where the code abbreviations along the *x*-axis are the same as those used in Table 5.2.

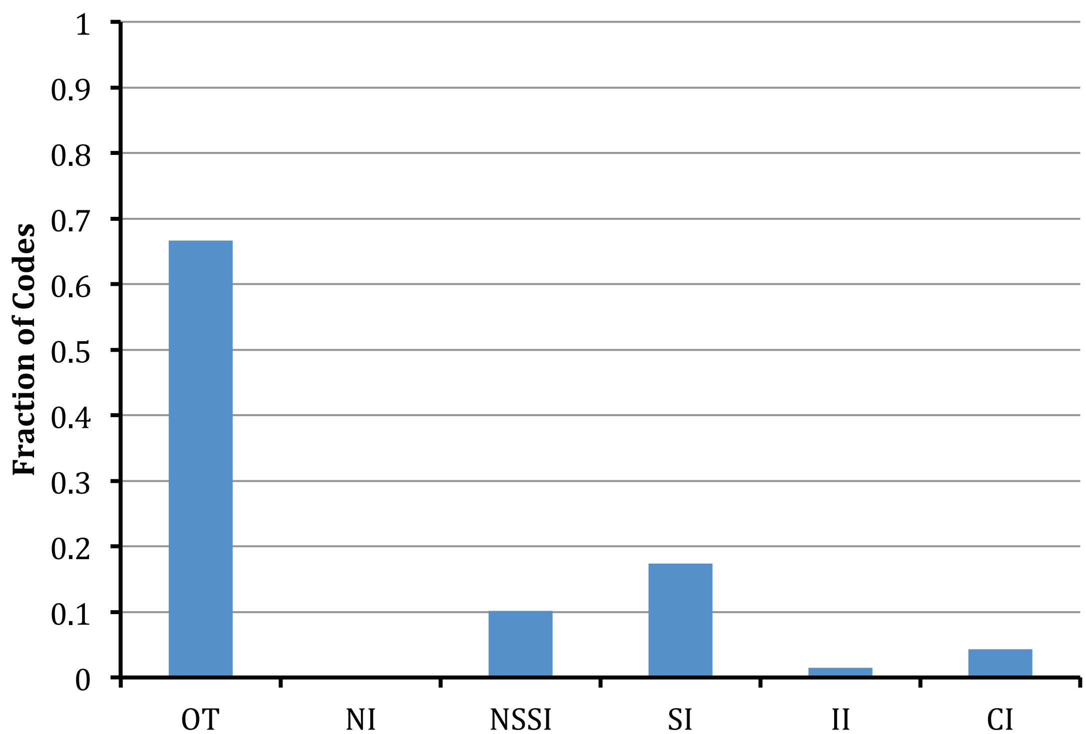


Figure 5.7 — Analysis of energy transfer representation task from Spring 2014. Code abbreviations along the *x*-axis are the same as previously defined in Table 5.2.

From this data we observed that just over 20% of representations included interactions between the solvent and the solute as indicated by the SI (17%), II (1.4%), and CI (4.3%) bars. Additionally, of the 20% that included these interactions, approximately 5% of representations included an intact solute into which the solvent molecules could collide (see the II and CI bars). This reflects previously reported findings that students rarely depict the dissolving process as involving the formation of interactions between the solvent and the undissolved solute even after viewing animations of the process (Abell & Bretz, 2018; Kelly & Jones, 2007; K. C. Smith & Nakhleh, 2011).

We next analyzed student responses to the SRA in formative and summative assessment settings, the results of which are shown in Figure 5.8. Again, the code abbreviations along the *x*-axis are the same as those used in Table 5.2.

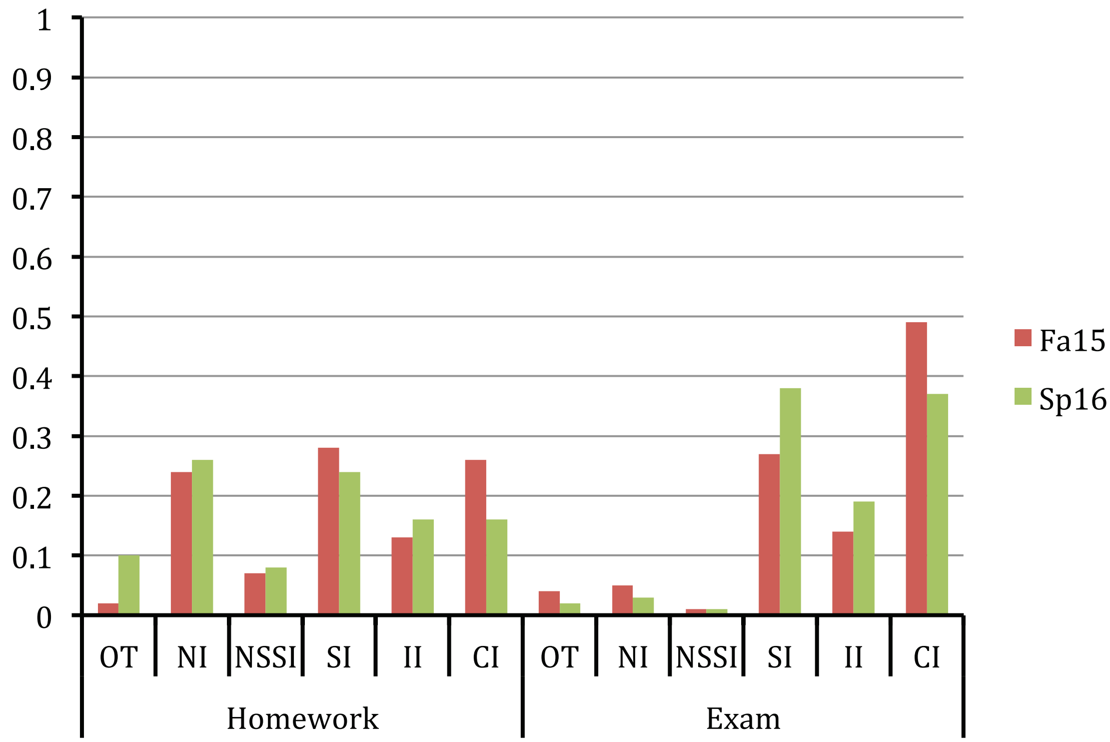


Figure 5.8 — Analysis of solution formation representation tasks from Fall 2015 and Spring 2016 as administered in formative and summative assessments. Code abbreviations along the *x*-axis are the same as previously defined in Table 5.2.

The large group of representations coded OT observed in the Spring 2014 cohort is not observed in the new assessment. More than half of representations produced in homework assessments were coded as either SI (28% and 24% for Fall 2015 and Spring 2016, respectively), II (13% and 16% for Fall 2015 and Spring 2016, respectively), or CI (26% and 16% for Fall 2015 and Spring 2016, respectively). That is, the percent of students who are representing in some way that the solvent and solute must interact is much higher in the more scaffolded task (the SRA).

Table 5.4 — Chi-square statistics comparing distribution of codes for representations of mechanism of solution formation in both homework and exam settings across cohorts. Significant differences are indicated by bold p-values

Assessment Type	Pearson Chi-Square	*df*	*p*-value	Cramer's V
Homework	128.574	10	**<0.001**	0.691
Exam	5.460	5	0.362	N/A

Chi-square analysis was performed to further investigate how students from the different cohorts represented the solvation process; these results are shown above in Table 5.4. These results indicate that the distribution of codes applied to student representations of the solvation process is not equivalent at the $p < 0.001$ level among the three cohorts for homework assessments ($\chi^2 = 128.574$, $df = 10$, $p < 0.001$). The Cramer's V value of 0.691 observed here indicates a strong association (Cohen, 1988) between the distribution of codes and the cohort. This was expected due to the large changes in the structure and content of the prompt used to elicit student representation of the solvation process.

The results from chi-square analysis of exam assessments administered in Fall 2015 and Spring 2016 ($\chi^2 = 5.460$, $df = 5$, $p = 0.362$) indicate that there is no difference in performance between the two cohorts in representing the mechanism of solution formation. We note this result since it indicates that the difference in demographics (relatively fewer freshmen and more sophomores in the Fall 2015 cohort) and in "sequence time" (Fall being "off-sequence" and Spring being "on-sequence") did not result in differential performance on the summative assessment task. Again, we suggest the content and structure of the CLUE curriculum (scaffolding of lecture, recitation, and homework activities) was successful in refining students' representations.

RQ3: What aspects of the task prompt are effective at eliciting evidence of student understanding?

Analysis of the responses to the "during" solution formation task from Spring 2014 (before revision), shows that nearly 70% of representations were either not at the atomic-molecular level or were uninterpretable as indicated by the OT bar to the left of the graph in Figure 5.7. Recall the wording used in the original assessment prompt:

> *Now draw a picture showing how the energy is transferred between the system and surroundings. Indicate what you are considering the system and what is the surroundings. In the black box explain why the temperature goes down (in the surroundings).*

Given the large number of instructions and concepts referenced before also asking students to provide an explanation, it is perhaps unsurprising that few representations depicted the atomic-molecular level while even fewer included interactions between solute (intact or otherwise) and solvent.

For this reason, the revised prompt provides three boxes to prompt students to think about the mechanism of solvation — explicitly focusing attention on atomic-molecular structure and interactions *before* the solution is formed, *while* the solution is forming, and *after* the solution is formed. By providing structure to the response area, the SRA serves to remind student to address the question: what is actually happening as the ions dissolve in solution?

Results presented in the previous sections show students were less successful depicting the mechanistic "during" step (as shown in Figure 5.8) than they were in representing the fully dissolved solution (see Figure 5.6). Despite this observation, representations with no solute-solvent interactions (codes OT, NI, and NSSI) were nearly eliminated in summative assessments. These data imply that representing the solvation process is much more difficult for students than representing the final aqueous solution. We interpret this to mean that understanding the process by which ions are separated from each other, where interactions are formed between the solvent and the intact solute, before and while the ionic bonding interactions in the solute can be overcome, is difficult for students. Indeed, the CI code was applied approximately half as often for the dissolving panel (49% and 37% for Fall 2015 and Spring 2016, respectively, see Figure 5.8) as for the dissolved panel (84%, 85%, and 91% for Spring 2014, Fall 2015, and Spring 2016, respectively, see Figure 5.6) in summative assessment tasks. While noting the less frequent occurrence of high-level representations of the solvation process, we also observe that representations with no solute-solvent interactions (10% and 6% occurrence for Fall 2015 and Spring 2016, respectively) were nearly eliminated in summative assessments responses to the SRA as indicated by the relative lack of OT, NI, and NSSI codes applied for exam assessment items. We also note that when students include an intact solute in their representation (as indicated by either II or CI codes), the CI code was two to three times more likely to be applied than the II code (Fall 2015: 49% CI, 14% II; Spring 2016: 37% CI, 19% II). This implies that it may be more difficult for students to include the intact solute in their representations than to both include the intact solute *and* show the solvent interacting with that intact solute.

Interestingly, when Kelly and Jones (2007) had students represent solvation before and after observing molecular level video animations of the process, only 7 of 18 students drew or wrote about solvent molecules pulling ions from an intact solute. While that research was conducted with a small sample size and used purposeful sampling to select students who were more descriptive on a screening task, the fraction of students who addressed interactions between an intact solute and the solvent (directly after viewing the simulation) was roughly equal to the student summative assessment performance in the current research study, using a representative sample of students from a large enrollment course.

<u>RQ4: How does the context of the task prompt (formative vs summative) affect student responses?</u>

Finally, we were interested in how student performance progressed between formative and summative assessment. While there are many ways in which performance on the high-stakes summative assessment might differ from that of the formative assessment (e.g. better understanding of content, higher effort level, or memorization for the exam) the question must first be addressed: was performance affected by the assessment setting? Before continuing, I remind the reader that while homework is reviewed during lecture in the CLUE curriculum (in general, and for the SRA specifically), written answer keys for these items are not provided for the students.

To obtain more information about student progress between formative and summative assessment, we compared codes applied to representations of the dissolving and dissolved portions of the SRA at for both formative and summative items. Chi-square analysis (shown below in Table 5.5) comparing distribution of codes applied to representations from homework and exam assessments indicates that none of the cohort's homework and exam performances were equivalent at the $\alpha = 0.05$ level. Values of Cramer's V indicate a medium association between distribution of codes and assessment type for responses to the SRA for both Fall 2015 and Spring 2016 cohorts. Spring 2014 and Spring 2016 cohorts also showed a medium association between assessment type for their representations of solvated ions. The Fall 2015 cohort showed a weak association between assessment type and code distribution. This is likely due the large fraction of students who represented the “dissolved” state with complete interactions (76%, see Figure 5.6) in the homework assessment.

Table 5.5 — Chi-square statistics testing for association between distribution of codes applied to formative and summative assessment responses for each cohort. Significant differences are indicated by bold p-values

Cohort	Representation	Pearson Chi-Square	*df*	*p*-value	Cramer’s V
Fall 2015	Solvation Process	24.723	5	**<.001**	0.352
Spring 2016		40.758	5	**<.001**	0.451
Spring 2014	Fully Dissolved Solution	16.210	5	**.003**	0.340
Fall 2015		11.138	5	**0.046**	0.236
Spring 2016		59.885	5	**<.001**	0.547

To further explore the effect of assessment setting on the representations students produced, bubble plots were created to show how each student represented the solvation process (Figure 5.9) and the fully dissolved aqueous solution (Figure 5.10) by comparing the codes for formative and summative assessments on the *x*- and *y*- axes, respectively.

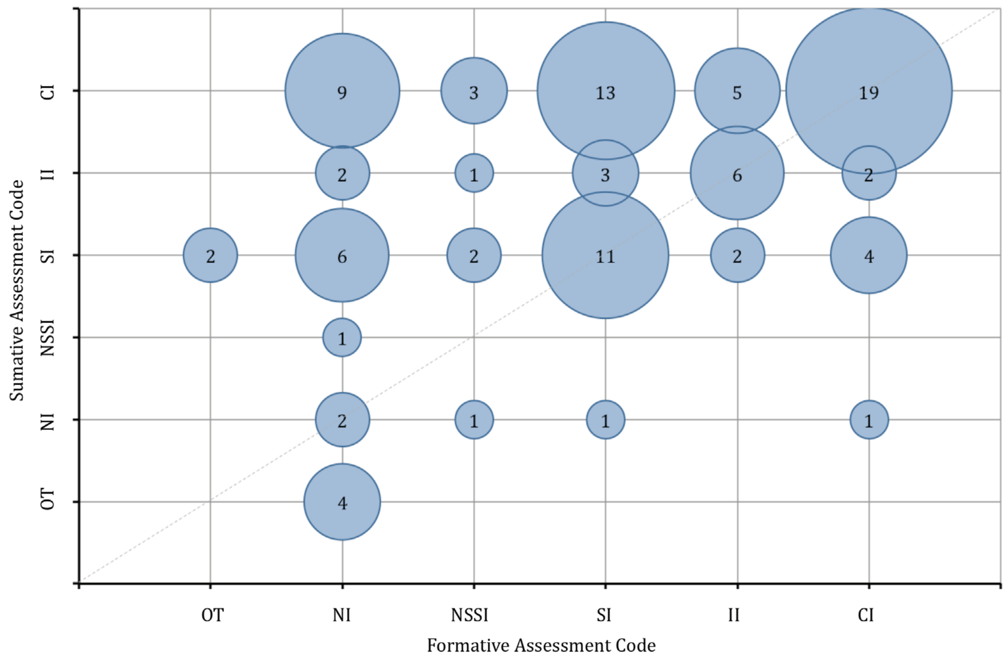


Figure 5.9 — Bubble plot of codes applied to student drawings in *dissolving* prompt of SRA formative and summative assessments administered in Fall 2015. Code abbreviations are the same as previously defined in Table 5.2. Relative bubble sizes are included for reference; the area of each bubble represents the frequency of each pair of codes.

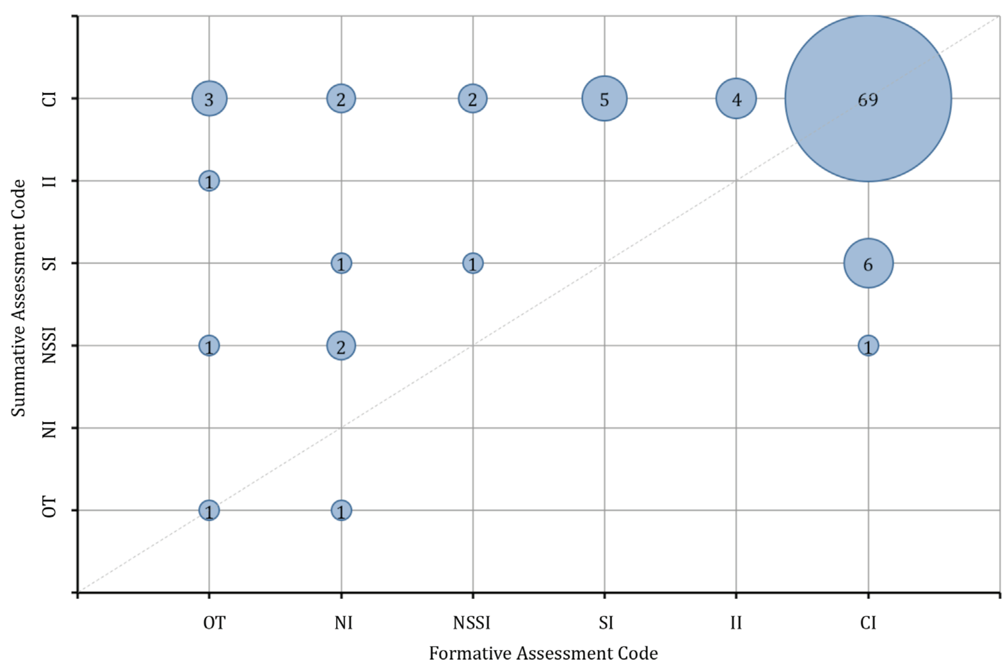


Figure 5.10 — Bubble plot of codes applied to student drawings in *dissolved* prompt of SRA formative and summative assessments administered in Fall 2015. Code abbreviations are the same as previously defined in Table 5.2. Relative bubble sizes are included for reference; the area of each bubble represents the frequency of each pair of codes.

In each of these figures, bubbles up and to the right signify students who have constructed representations featuring more complete interactions. For instance, in Figure 5.9, 19 students' representations of the dissolving process showed interactions between the solvent and an intact solute in both formative and summative assessment tasks as indicated by the bubble at the extreme top right (CI on both axes). Similarly, in Figure 5.10, 69 students' representations featured solvated ions in both formative and summative assessment tasks as indicated by the bubble at the extreme top right (CI on both axes). Note that students whose representations have the same use of interactions in summative and formative assessment tasks will be indicated by bubbles on the main diagonal represented by a dashed line in each bubble plot. Students whose representations were more sophisticated on summative than on formative assessments are indicated by bubbles above and to the left of the diagonal.

From the data in Figure 5.9 we can see that almost all of the students produced equally or more appropriate representations on the summative than the formative. Only 15 of the 100 students in the sample produced representations on the summative assessment containing fewer interactions than on the formative assessment for the more difficult dissolving panel of the SRA. Figure 5.10 shows that even fewer (8 of 100) students used less sophisticated interactions in their representations of the fully dissolved solution on the summative assessment task than on the formative assessment task. In fact, with the exception of students whose formative assessment representations were already coded as CI, only nine students did not use more interactions in their exam assessment representations than on homework.

As seen previously, students in the current study were much more likely to represent fully dissolved solutions with correct interactions than they were to represent the dissolving process with complete interactions. Although students appear to be less successful in representing the more complex process required for solutions to dissolve, the finding that students either maintained or increased the use of interactions between the solute and solvent from homework to exam assessments is encouraging.

There are many possible explanations of these findings. The first possible explanation of students' increased performance on summative assessment tasks is that they understood the material better, and were therefore better able to represent the solvation process and the dissolved aqueous solution. It has been suggested that meaningful practice with scientific representations and conceptual models, such as the worksheets students complete during recitation sections (see Figure 4.1), can help remind students of the important features to include in their own representations (National Research Council, 2007). While we cannot be certain, the increase in sophistication of representation of interactions by the summative assessment task seems to provide additional evidence that the CLUE curriculum is successfully able to help students improve their representations of the atomic-molecular level solvation process.

It is also possible that students simply tried harder on the summative assessment. Recent research investigating the relationship between performance on low- and high-stake assessments suggest that participants who put forth "even minimal effort" perform similarly well in both low- and high-stakes settings (Attali, 2016 p. 1056). While we cannot rule out the possibility that some participants did not meet the "minimal effort" criteria, the observation that students produced any representations at all given the relative difficulty of drawing with a computer mouse or trackpad, especially as compared to the pencil and paper summative assessment, seems unlikely.

A final possibility we consider here is that students were able to memorize an appropriate, or at least more sophisticated, representation in time for the exam. We cannot rule this out, although students' relative success (compared to literature reports) on the formative assessment tasks seems to indicate that student might not have felt it necessary to resort to rote memorization. We note that the summative assessment items were administered on the first exam of the semester, although it is not clear what effect that might have had on students' motivation to memorize.

Conclusions

An assessment was designed to probe student understanding of the mechanistic process by which aqueous solutions of ionic salts are formed as well as the molecular level structure of these aqueous solutions. Analysis of responses to this assessment in formative and summative contexts indicates that most students in the CLUE curriculum can successfully represent aqueous solutions as isolated ions that independently interact with solvent molecules. This is especially noteworthy given the numerous reports of student difficulty in similar tasks (Abell & Bretz, 2018; Ebenezer, 2001; Herrington et al., 2017; Kelly & Jones, 2007, 2008; K. C. Smith & Nakhleh, 2011; K. J. Smith & Metz, 1996). Students are less successful representing the interactions that must take place between solvent molecules and the intact solute during the solvation process. This finding was not unexpected, as solvation requires the accounting of many concerted processes. Students' success in representing the solvation process on a summative assessment task was similar to those seen by Kelly and Jones (2007) for a much smaller group of students after viewing molecular level video animations of the solvation process.

However, even though representing this complicated set of events was difficult for students, analysis of summative assessment data show that nearly all students included interactions between a solute and the solvent in their responses to both dissolving and dissolved portions of the SRA. This is encouraging since the dissolving process *requires* that the solvent and solute form attractive interactions in order to separate ions from each other and overcome the pre-existing ionic bonding interactions present in the ionic salt.

Finally, it is imperative that assessment prompts be structured in such a way that is meaningful to students to elicit responses at an appropriate level of detail to exhibit mechanistic reasoning. To support this premise, we observed results from students in the Spring 2014 cohort and compared to results from Fall 2015 and Spring 2016 cohorts. All three cohorts were able to successfully represent dissolved solutions; the distributions of codes applied to these representations produced on summative assessments were statistically equivalent. There is no reason to think that the Spring 2014 cohort could not also have been similarly successful in representing the dissolving process had the prompt been properly structured. Furthermore, we argue that the large fraction of "Off-Task" responses supports this since it implies that students either did not interpret the prompt to require a representation of the dissolving process at the atomic-molecular level or that they were not capable of doing so. Based on their success in drawing solvated ions in a fully dissolved solution, we do not believe that Spring 2014 students were incapable of constructing atomic-molecular level representations.

Inherent in the call to structure assessment prompts in a way that is meaningful to students is the need to disaggregate the things we want students to do so that reading the mind of the assessment designer is not the most important aspect of the task. By designing tasks that are clear in their expectations, we can increase the likelihood that students' responses will reflect what they know and can do, rather than just what they thought was the most appropriate way to respond to a potentially ambiguous, unclear, or confusing prompt. As educators and education researchers, we accept that we can never fully know what students know, but we attempt to elicit evidence of what they know through well-structured assessments. However, this research also suggests a corollary: just because a student does not perform on an assessment does not mean that they *cannot* perform. It might merely mean that the task did not adequately signal to students what specific performances would demonstrate understanding or mastery.

Implications

While representing the mechanism of solution formation appears to be difficult for students, we observed that nearly all representations included solute-solvent interactions. Furthermore, in responses that included a representation of an intact solute, students were two to three times more likely to depict the process as occurring via interactions between the solvent and that intact solute. We believe that supporting students to think about the requirements of solution formation, namely that there must be an intact solute present, could facilitate students in representing the solvation mechanism.

Given how successfully CLUE students represented aqueous solutions, we believe that the repeated explicit references to connections between molecular structure, interactions, energy, and properties across concepts supports students' ability to depict the molecular-level interactions present in solutions. Previous work in our group has shown that students in the CLUE curriculum are particularly well equipped to draw and use structures to make predictions about properties (Cooper et al., 2012). Instruction on solutions builds upon this foundation by explicitly drawing on students' understanding of interactions and intermolecular forces to explain why, for instance, ethanol is miscible in water, but not hexane. Because electrostatic and bonding interactions (and particularly intermolecular forces) are used throughout the course, students only need to understand the role that these familiar concepts play when applied to solutions. The success that these students had in this research is further evidence that the structure of the CLUE curriculum, including the explicit linking of new material to prior knowledge, can support student success as they encounter historically difficult content.

Limitations and Future Work

There are two primary limitations present in the current study. The first concerns the student population. Only students enrolled in the CLUE curriculum from a single university are included in these results. It will be important to investigate if and how the range and distribution of interactions used in representations varies for different populations of students as CLUE is adopted at more (and more diverse) institutions.

The second consideration is that this analysis only considers representations of interactions present in student drawings. The primary goal of this study was to characterize evidence from student representations that was indicative of mechanistic understanding of solutions and the solvation process. While energy and entropy certainly contribute to this process, those concepts are more difficult to express in drawings, and were therefore not included in this analysis. Further characterization of students' understanding of solutions and solvation will necessarily capture evidence of students' understanding of the energy changes (especially as related to interactions) and the relationship between enthalpy, entropy, and solubility.

Finally, another extension of the current work is related to the principles of assessment design and scaffolding used to develop the SRA. Scaffolding was included in the assessment task by providing three separate sections in the response area. This was done to explicitly call attention to potentially overlooked components of the process, namely the interaction of the solvent with the intact solute, as suggested by research on scaffolding and assessment design (Reiser, 2004; Reiser & Tabak, 2014). One aspect of scaffolding that is often neglected is the expectation that the scaffold itself fade away over time as the learner gains expertise, ultimately leaving her able to complete the task independent from assistance previously provided by the scaffold (Sherin, Reiser, & Edelson, 2004). A future project to characterize the durability of student understanding would likely involve removing the three prompt scaffolding in stages. One way to implement fading would be by first removing the vertical lines delineating the separate panels (as a first stage of fading) followed by removing the "Undissolved", "Dissolving", and "Dissolved" headings. Analysis of student representations at each stage of fading should provide evidence of more or less expert-like understanding of the solvation process.

CHAPTER 6 — HOW DO STUDENTS EXPLAIN A TEMPERATURE CHANGE THAT ACCOMPANIES SOLUTION FORMATION?

In the introduction to the previous chapter, a fundamental goal of chemistry education – to support students to understand how energy changes, interactions, structure, and stability at the submicroscopic-level act as levers that govern everyday macroscopic phenomena – was presented. Here I argue that another fundamental goal of chemistry education is to develop analysis tools and methods to obtain evidence of (or related to) student understanding and learning.

Because chemistry is concerned with the relationship between macro-scale properties and submicroscopic energy, bonding, and interactions it can be difficult to obtain sufficient evidence from a single assessment task to indicate how deeply a student understands (and is able to use) the relevant disciplinary content. Previous work in the Cooper group has used a combination of representational and explanation or argumentation tasks to provide a more complete picture of student understanding of London dispersion forces (Becker et al., 2016), intermolecular forces in general (Cooper et al., 2015), and acid-base reactions (Cooper et al., 2016).

With these thoughts in mind, this chapter investigates an explanation prompt that was paired with the SRA representation task. The explanation prompt asked students to explain a given temperature change that occurred when an ionic salt dissolved in water. The iterative development of the explanation task (subsequently referred to as the Thermal Energy in Solvation Assessment, or TESA) was previously described in Chapter 4. Briefly, both versions of the TESA were intended to elicit students' understanding of the mechanism by which energy was transferred at the molecular level and subsequently explain why the temperature decreased by using the energy transfer mechanism and ideas related to the strength of interactions between the solute and the solvent that were either formed or overcome as necessary. An explanation of this phenomenon would likely leverage *collisions* to transfer energy, a comparison of both interactions formed and overcome, and an explicit treatment of the energy flow resulting from the changed interactions that also explains the observed change in temperature.

In addition to the components mentioned above, a *causal mechanistic* explanation would identify and utilize entities and causal factors that are at least one grain size smaller than that of the phenomena (Krist et al., 2018); these causal factors (and the entities of which they are composed) generally initiate the sequence of events that compose the explanation (Braaten & Windschitl, 2011). For the example of sodium chloride dissolving in water, the most likely causal entities would be the partial positive and negative charges localized on the hydrogen and oxygen atoms in water (for the solvent) and the positively charged sodium cations and negatively charged chloride anions (in the intact solute). The attraction between the entities (that is, the causal factor) in the solvent (e.g. the $\delta+$ hydrogen in water) and those in the intact solute (e.g. the negatively charged chloride anion) would result in collisions (which transfer energy into the undissolved salt) and formation of interactions that would result in hydration of solute ions ultimately resulting in concerted removal of sodium and chloride ions from the intact solute by the water molecules. So far, this paragraph has provided a causal mechanistic account of the solvation process. In order to construct the explanation, this account would additionally require comparison of both interactions formed and overcome, explicit treatment of the energy flow resulting from the changed interactions, and ultimately link the net energy flow caused by the breaking and forming of solute-solute, solvent-solvent, and solute-solvent interactions to the observed macroscopic temperature change.

The types of explanation we want students to be able to construct and use are important, particularly in chemistry, because they serve to connect observable phenomena to structure, properties, energy, and change at the atomic-molecular level. Additionally, these highly detailed and structured explanations can provide a starting point for students to begin to generalize from a specific explanation of a single phenomenon more broadly into a more theory-like understanding (National Research Council, 2012).

The rest of this chapter describes the development of a coding scheme to characterize student explanations, results obtained from applying the coding scheme to student responses from three versions of the explanation prompt, and implications of these results. Discussion of the coding scheme development process demonstrates some of the difficulties inherent in trying to characterize explanations constructed by novice learners. It is important to call attention to the assessment setting of the current chapter; these explanation tasks were administered as part of a larger formative assessment activity (the development of which was previously described in Chapter 4; the final revised version of the complete formative assessment activity as administered in the beSocratic system is presented in Appendix C) that students completed for homework after the first of two lectures designed to specifically address aqueous solutions of ionic salts. Given the complicated nature of the solvation process and the (likely) novice level of students' understanding at the time of the assessment, it is expected that students will have some difficulty constructing well-structured and complete causal mechanistic explanations of the phenomenon.

Therefore the focus of the final coding scheme is not some sort of holistic ensemble measure of success. Instead, the focus of code development was to describe and capture evidence from student responses that could indicate that students were (or were not) thinking mechanistically about the solvation process. With these considerations in mind, the coding scheme that was developed in this work is ultimately focused on characterizing students' use of interactions in their explanations.

The research questions that guided this study were:

1. How do students use ideas of interactions while explaining a temperature change?
2. What aspects of the task prompt are effective at eliciting evidence of student understanding?

Methods

Student participants

As previously mentioned, student participants in this research were enrolled in the second of a two semester general chemistry sequence at MSU taught using the CLUE curriculum (Cooper & Klymkowsky, 2013a) from Spring 2014, Fall 2015, Fall 2016, and Spring 2017 semesters. From these populations, cohorts of 75, 100, 83, and 82 students were randomly selected; demographics of each cohort are shown below in Table 6.1. The demographic data for each cohort are not statistically different from those of the populations from which they were selected.

Table 6.1 — Gender, class standing, ethnicity, and common majors for Spring 2014, Fall 2015, Spring 2017, and Fall 2016 (replication) cohorts

Demographics	Spring 2014 (N=75)	Fall 2015 (N=100)	Spring 2017 (N=82)	Fall 2016 (N=83)[a]
Gender	52% Female 48% Male	60% Female 40% Male	56% Female 44% Male	62% Female 38% Male
Class Standing	79% Freshman 16% Sophomore 5.3% Upperclass	16% Freshman 49% Sophomore 35% Upperclass	41% Freshman 33% Sophomore 27% Upperclass	13% Freshman 52% Sophomore 35% Upperclass
Ethnicity	77% White 9.3% Asian 13% URM	66% White 9.0% Asian 25% URM	65% White 9.6% Asian 25% URM	63% White 8.0% Asian 29% URM
Common Majors	24% Premedical 16% Human Biology 7.9% Kinesiology	16% Human Biology 6.7% Premedical 6.0% Kinesiology	19% Human Biology 13% Premedical 6% Neuroscience	20% Human Biology 9.7% Kinesiology 6.8% Mathematics

a. Student sample from Fall 2016 was used to replicate results observed for the Spring 2017 sample as discussed below. Placement of the Fall 2016 to the far right of the table was intentional to indicate its use as a replication sample

Thermal Energy in Solvation Assessment

Students' ability to explain a given temperature change that occurred while a solution formed was assessed using the TESA previously described in Chapter 4. The TESA was part of a larger formative assessment activity centered on the mechanism, energetics, and entropic and enthalpic contributions to solution formation. Examples of initial and revised versions of the TESA (TESA v1 and TESAfinal) used in formative assessments are shown below in Figure 6.1. (Please see Chapter 4 for a discussion of the development of the TESA, and Appendix C for the full formative assessment activity). The revision from initial to final version of the explanation prompt was influenced by the Explanation Tool, which was originally created to help teachers identify explanations of increasing complexity from *What*, to *How,* and ending with *Why* (Braaten & Windschitl, 2011). By using these categories of explanation as prompts we were able to separate out relevant components of the explanation (similarly to how the SRA is divided into three snapshots) and structure explanation prompts so that difficulty and complexity slowly increased. An additional benefit of the three prompt sequence is that it leverages a scaffolding strategy that calls attention to components of the phenomenon that students may have forgotten or taken for granted (Reiser, 2004).

Figure 6.1 — First revised (top) and final revised (bottom) versions of the TESA, when administered as a formative assessment task

It is important to make two comments before continuing. The first is that, while the TESA is completed as part of a larger homework activity for the formative assessment data presented below, students are not provided with a written answer key to homework tasks. This is true throughout the CLUE curriculum in general, and specifically for the TESA. The second is that the specific ionic salt used in the TESA prompt is not always constant; while a binary salt is always used, the exact salt and its associated heat of solvation are variable. Because students are not asked to explain aspects of the solvation process related to entropy in the TESA this is not considered a limitation.

Analysis

Student explanations were analyzed in an iterative process utilizing multiple strategies. Initial codes were developed using a combination of codes observed from the previously discussed student interviews (see Chapter 4) and an initial coding approach utilizing constant comparison techniques to ensure consistency of coding (Corbin & Strauss, 2008). Subsequent analysis focused on consolidating the initial open codes to develop themes observed in student responses. Additional coding schemes were developed to leverage results of semi-structured interviews to characterize students' use of energy or interactions in their explanations.

Initial Coding

Initial coding provided a starting point to describe the types of things students did or included in their responses. These codes were not mutually exclusive, but no code was applied more than once to any student's response. Generally, codes described the presence (and nature) of mechanisms, process descriptions, single component explanations, explanations including a comparison of components, and unclear or uncodable responses. See Table F.1 in Appendix F for a complete listing of initial codes generated in this phase of analysis.

Axial Coding

Axial coding refined and consolidated the previously developed open codes. The same main categories of codes were used (use of mechanism, single component, comparison of components, descriptive, and unclear or otherwise uncodable). Each category was divided into "canonical" and "noncanonical" codes. As with initial codes, categories were not mutually exclusive, but no code was applied more than once to any individual response.

Coding for components

Previously developed axial coded were further refined to three categories describing the presence of collisions, the nature of interactions included (balance or single), and the causal factor resulting in the observed temperature change (energy or only interactions). Again, categories were not mutually exclusive, but no code was applied more than once to any individual response.

For this coding scheme, the most complete response would be one that leverages *collisions* to transfer energy, considers the *balance* of interactions that are overcome and those that are created, and uses the *energy* flow of making and breaking interactions to explain the overall temperature change. Such an explanation would have been coded with <u>C</u>ollisions, <u>B</u>alance, and <u>E</u>nergy.

Coding for energy

Following the implementation of a coding scheme to characterize students' use of interactions in representing the solvation process (see Chapter 5), an analogous coding scheme designed to target the CLUE core idea of energy was developed to characterize student responses to the TESA. Because this scheme was designed primarily to capture the use of energy ideas, other possible components of student explanations were deemphasized. Initial versions of this coding scheme contained five mutually exclusive categories describing students' use of energy ideas to describe the temperature change that accompanied solution formation as summarized below in Table 6.2. The following discussion describes the coding scheme and includes exemplars to illustrate the ways energy was used in student explanations. While the version of the TESA shown earlier (as used in formative assessments) asks students to explain why the temperature of the system decreases, these codes are all also applicable for a system in which the temperature increases when the salt dissolves. The examples shown below are from a version of the TESA in which lithium iodide, the solvation of which is an exothermic process, was used.

Table 6.2 — Summary of codes generated to describe students' use of energy ideas to explain the temperature change accompanying solution formation

Code	*Description*
Balance (correct)	Energy is used to describe both forming and overcoming interactions and the overall temperature change is described as resulting from the net energy flow of the component steps
Balance (nonspecific)	One of the treatments of breaking or forming interactions is ambiguous such that energy flow required to change an interaction is not obvious
Balance (incorrect)	One or both of the treatments of breaking or forming of interactions are explicitly incorrect
Single component	Only one change in interactions (and its corresponding energy change) is presented as causing the observed temperature change. Note that the energy flow accompanying breaking or forming of interactions does *not* have to be correct. The limiting factor is that only one change (breaking or forming interactions) is applied to the explanation of the cause of the observed temperature change.
Off-task	No reference to how components of explanation result in or cause the observed temperature change.

The most sophisticated use of energy was described by the "Balance (correct)" code. These responses included a discussion of (*i*) interactions broken or overcome, (*ii*) interactions formed, and (*iii*) an explicit comparison resulting in a net energy flow corresponding with the observed temperature change. An explicit reference to energy was required for this code to be applied; only referencing strengths of interactions formed or broken was not sufficient.

> "The temperature increases because the formed interactions [are] at a lower energy level than the broken interactions. More energy is given off by the formation of interactions than used by the breaking of interactions."

The above response was coded "Balance (correct)" because it refers to forming interactions releasing energy ("more energy is given off by the formation of interactions"), breaking interactions requiring energy ("… than used by the breaking of interactions"), a comparison ("formed interactions are at a lower energy level that the broken interactions"), and treats energy as causal for the temperature change ("the temperature increases because… more energy is given off… than used").

The "Balance (nonspecific)" code describes explanations that reference a balance of interactions, but do not explicitly refer to the energy of forming and breaking interactions.

> "The temp increases because overall the interactions between the solute and solvent were stronger than solute-solute and solvent-solvent interactions. When you form new bonds/interactions <u>energy is released</u> heating the surroundings." (emphasis in original)

In this example, the temperature change is caused by a difference in *strength* of interactions ("overall the interactions between the solute and the solvent were stronger than the solute-solute and solvent-solvent interactions") and the energy change of forming interactions is referenced ("when you form new bonds/interactions energy is released"). However, the *energy* required for breaking and released when forming interactions are not compared. While it may be obvious to the expert chemist that the amount of energy required or released when breaking or forming interactions is related to the strength of those interactions, it is not always true that novice chemists are necessarily relating energy requirements to the strength of interactions when writing about one but not the other.

The “Balance (incorrect)” code captures responses that have attempted to explain the temperature change by comparing interactions, but have failed to correctly characterize the energy changes accompanying one or both of these processes.

> “The temperature increases when the strong covalent bonds are broken and replaced with weaker hydrogen and ionic bonds. More energy is released while breaking bonds than is absorbed while creating new bonds.”

There are many incorrect statements in the above example. No covalent bonds are broken when an ionic salt dissolves. Likewise, no ionic bonds are formed. Furthermore, breaking bonds does not release energy and energy is not absorbed when bonds form. However, this explanation does compare the two processes of breaking and forming interactions, which is the only requirement for the code to be applied.

When only one component is used, as in the example below, to explain the temperature change the “Single” code is applied. This code does not require that the energy flow accompanying breaking or forming is correct. The key feature is that only one process is considered, and that energy is related to the temperature change in some way as seen in the example below.

> “When you are making bonds, energy (heat) leaves the system and goes into the surrounding causing the temperature to increase.”

In this explanation, only the forming of “bonds” is used to explain the increase in temperature. It is important to note that explanations that only included one component to explain the temperature change, whether breaking or forming interactions, were not further parsed to capture additional detail (as was done in the “balance” codes discussed above). Similarly to how interactions between the solute and the solvent were prioritized in Chapter 5, students' use of energy was prioritized in these codes. Because these "single component" responses did not address both contributions to the overall energy change they necessarily included a less complex treatment of energy than the family of "Balance" codes.

The final code in the scheme ("Off-task") is applied to responses that have no reference to how the components of the explanation result in or cause the observed temperature change, restate the prompt, or are otherwise off topic.

Following development of these codes, the reliability of the coding scheme was evaluated by training an independent coder and comparing codes assigned to student responses. This iterative process of coding, comparison, and code refinement was repeated for multiple cycles. Ultimately, the reliability of this coding scheme was unable to be confirmed, as shown by the maximum observed percent agreement of 63% with a Cohen's kappa of 0.52 indicating only moderate agreement (Landis & Koch, 1977). We attribute the lack of reliability observed with this coding scheme to the many different ways students could talk about energy. These results appear to be a more extreme example of the difficulty of coding student explanations (relative to drawings) documented by Cooper et al. (2015) in their work on student understanding of intermolecular forces.

Coding for evidence of interactions

Previous work (see Chapter 5) analyzing students' drawing of the dissolving process has shown that while students are largely successfully drawing solvated ions in solution, they have difficulty depicting the process of solvation at the atomic-molecular level. Few representations of the solvation process included solvent molecules interacting directly with the intact solute which would indicate an understanding of the mechanism underlying solution formation.

This phase of analysis was intended to see if there was a similar disconnect in students' explanations when they were asked to identify the energy transfer mechanism (i.e., collisions) and explain the temperature change that occurs with the successful dissolving process. While the TESAv1 prompt (see Figure 4.9) does not explicitly ask students to describe the solvation process that they had just previously drawn, a description of how and why the temperature changes will include the interactions overcome and formed. Indeed, simply stating that collisions occurred between the solvent and the solute to transfer energy was considered an interaction.

In order to focus coding on characterizing evidence that students understand or are thinking mechanistically about the solvation process, their use of interactions was prioritized over entropic and enthalpic factors. Additionally, very little emphasis was placed on the "correctness" of explanation components; the behavior that these codes were intended to capture was that of using interactions in a way that is causal to the intact solute dissolving. An additional benefit of this decision is that anticipated difficulties students might have had, perhaps related to the energetics of breaking and forming interactions, did not overwhelm the productive ways that interactions were used in their explanations.

Developing the coding scheme to describe students' use of interactions between the solvent and the intact solute progressed through a number of iterative steps. These codes were developed to characterize evidence that students were explaining the temperature change in a *mechanistic* way. The key feature in the final coding scheme was evidence that students either were or were not explicitly accounting for these solvent-intact solute interactions (which are also referred to as the mechanistic step) that are often missing in the "dissolving" portion of students' representations of the mechanism of solvation formation (recall from Chapter 5 that the mechanistic step is the difference between "Incomplete Interactions" and "Complete Interactions" representations of the process of dissolving). A summary of the final codes developed is shown below in Table 6.3,

Table 6.3 — *Coding for Interactions* code summary. "Present" and "Absent" code categories refer to whether interactions between the solvent and an intact solute are in explanations

Code Category	Code	Description
Present	Explicit	Explicitly refers to what part of the solvent interacts with what part of the intact solute
	nonSpecific	Interactions between the solvent and the intact solute are described, but does not specifically refer to what part of the solvent interacts with what part of the intact solute
Absent	nonIntact	Refers, explicitly or implicitly, to interactions **BUT** only refers to interaction where solute is already dissolved
	None	No reference to interactions in student's response

The first iteration only included "present" and "absent" codes to describe whether students did or did not discuss interactions. This was quickly modified as more variety in responses was observed than could be adequately captured using just these two codes. The next version divided the "present" codes into an "explicit – specific" (ES) and "implicit – general" (IG) category. This was done to capture the difference in detail provided in responses. The ES code was applied when explicit detail about the interactions being formed was provided:

> "As the Na and Cl are broken they begin to be attracted to either the positive H or negative O in the water molecule. The ions then begin to form bonds with the H and O in the water."

In this response, the student is referring to specific parts of the solute that will form interactions with specific parts of the solvent.

Responses coded as IG included references to interactions formed as the salt dissolved, but were limited in the detail provided:

> "Polar water molecules come in and ion-dipole interactions are formed between water and ions."

This response indicates that interactions are formed, but does not provide enough information about these interactions to determine where the interactions were or why they formed.

Responses given a general "absent" code indicate that there was no mention of any newly formed interactions:

> "During the dissolving process an endothermic reaction is occuring because the ionic bonds of NaCl are breaking. Energy is needed when bonds break so the energy is leaving the surroundings (H2O) and being used to break the ionic bonds of the NaCl."

In this response, the specific interactions that are overcome are discussed ("the ionic bonds of NaCl are breaking"), but there is no reference to the formation of any new interactions.

The next modification to the coding scheme was to split the "absent" code and add a category named "something formed" for stating that new interactions were formed, *or* for naming or describing the type of interaction that was formed:

> "Then the interactions the solute-solvent require releasing a certain amount of energy to the surroundings when formed."

From the response, we observe that interactions were formed, but no further information is provided about these interactions. While this code was useful in further developing the overall coding scheme, those revisions made it redundant; "something formed" is therefore no longer used.

The final addition (and perhaps most obvious in hindsight) was the implementation of a "nonintact solute" (NS) code. Similar to the distinction between upper levels of drawing coding where the inclusion of interactions between the solvent and an intact solute indicates a more sophisticated response to the prompt, explanations that clearly indicated that solvent molecules interacted directly with intact solute are more indicative of the type of mechanistic detail we want students to understand. These NS responses indicate that interactions were formed, but imply that these interactions were not formed until *after* the previous interactions have been overcome (i.e. – after the lattice had been broken apart). Reference to the formed interactions may be either explicit or implicit with respect to the specific ions and portions of solvent molecules involved (in fact, the interactions referenced do not have to be correct; the only consideration was that the interactions formed after the original interactions were overcome). While some examples are rather ambiguous, these responses will usually have a sequence word in the response such as "then" or "next" indicating that the original interactions were overcome before any new interactions could form.

> "The interactions in the solute and solvent require a certain amount of energy to be broken. Then the interactions the solute-solvent require releasing a certain amount of energy to the surroundings when formed."

This example was coded as NS because the response states that there is a sequence the change in interactions: interactions are *first* overcome, *then* solute-solvent interactions can be formed.

The finalized set of codes developed to evaluate students' use of interaction in their explanations of temperature change during the solvation process is shown in Table 6.3 above. General categories of codes indicate whether the response invoked the idea of interactions between the solvent and the intact solute ("Present") or not ("Absent"). Individual codes then described whether students indicated the specific entities that were interacting ("Explicit"), if a general description was given that the solute was intact when interactions between the solute and solvent were formed ("nonSpecific"), if the solute was already dissociated when interactions between the solute and solvent were formed ("nonIntact"), or if there were no interactions formed between the solvent and any solute ("None").

For more details, including extended explanations of code definitions, see Appendix G for the complete codebook describing the coding scheme. Once the coding scheme was finalized, the reliability of codes was investigating by training an independent coder and comparing codes assigned to student responses. Independent coding for students' use of interactions in explanation tasks resulted in 93% agreement with a Cohen's kappa of 0.90 indicating near perfect agreement (Landis & Koch, 1977). We attribute the relative ease of demonstrating reliability in this coding scheme, especially relative to the "Coding for Energy" codes described in the previous section, to students' experience using interactions between atoms and molecules throughout the CLUE curriculum. By the time students encounter the solutions and solvation they have been identifying, representing, and explaining intermolecular forces to explain properties across a wide range of substances for nearly an entire semester. We suggest that this facility with interactions resulted in the use of more coherent language when describing interactions that was therefore easier to characterize.

Results and Discussion

Following development of the coding scheme to characterize students' use of interactions in their explanations of the temperature change that accompanied solution formation, analysis of student responses focused on formative assessments. This decision allowed several affordances. First we felt students would be more likely to respond in a way that reflected their authentic understanding of the process, rather than responding predominantly in an effort to maximize the points earned on an exam question (i.e. the canonical "brain dump" or "shotgun strategy" of test taking). Secondly, focusing on formative assessment items allowed coding to place very little emphasis on whether the individual explanation components were correct or incorrect. It was anticipated that this would allow the coding to capture the productive ways that interactions were used in explanations without being overwhelmed by other difficulties (e.g. related to energetics) that might be present. The following sections describe and discuss these results.

<u>RQ1: How do students use ideas of interactions while explaining a temperature change?</u>

Responses to the original explanation prompt administered in Spring 2014 (shown previously in Figure 4.3d and reproduced below in Figure 6.2) were analyzed to formally investigate early impressions that the prompt was not eliciting evidence of student's understanding of the mechanism by which energy was transferred during the solvation process. The results of this analysis are shown below in Figure 6.3; note that the "Absent" and "Present" categories on the *x*-axis refer to the absence or presence of interactions between the solvent and the intact solute. The left bar is composed of responses that either did not invoke collisions or formation of solvent-solute interactions at all (shown in purple), or only after the solute dissociated (shown in green).

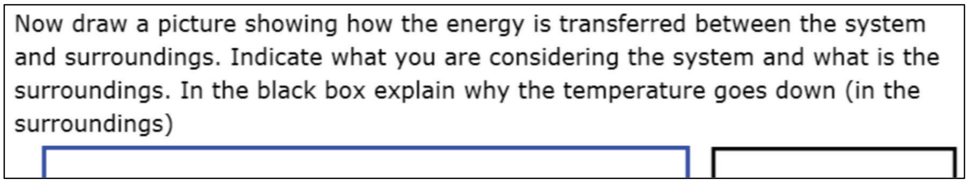


Figure 6.2 — Energy transfer mechanism prompt from initial formative assessment activity administered in Spring 2014

From the data shown in Figure 6.3 it is clear that students did not include ideas of interactions or collisions between the solvent and the intact solute in their explanations. No responses explicitly described the formation of interactions between specific ions and atoms in the solute and solvent molecules respectively; only 3% included general ideas of collisions or interactions forming between the solvent and the intact solute (see the red bar in Figure 6.3). This indicates that either (*i*) students do not understand the energy transfer mechanism as requiring collisions or interactions between the solvent and the intact solute or (*ii*) this prompt did not sufficiently elicit students' understanding of the energy transfer mechanism.

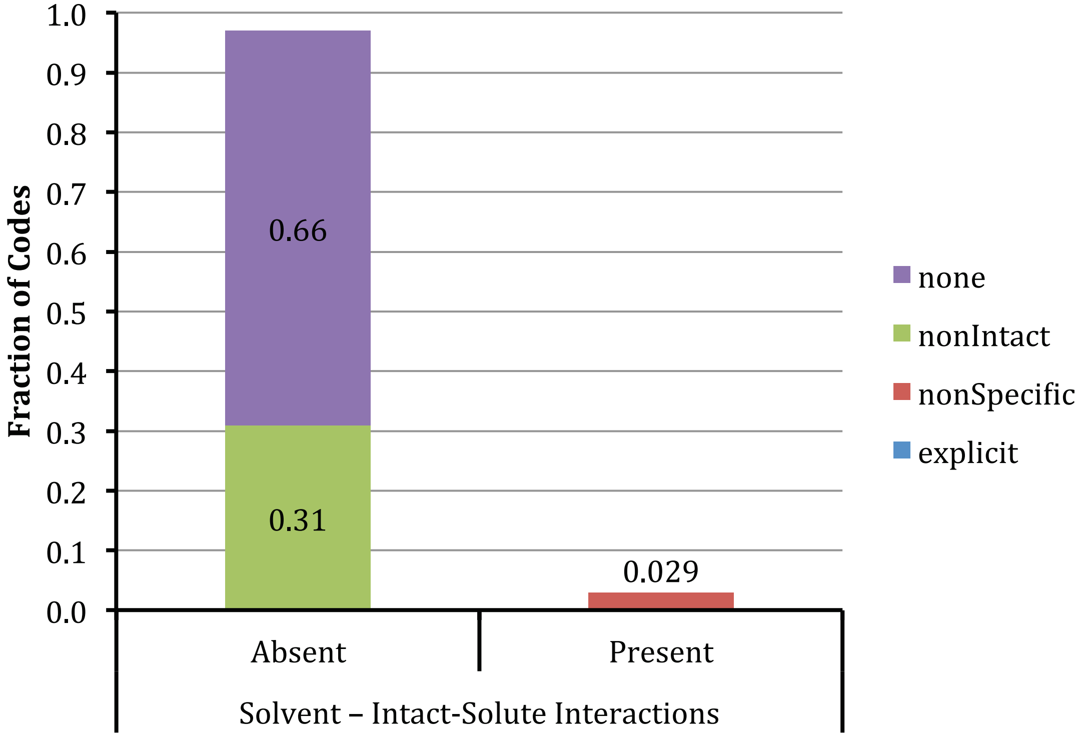


Figure 6.3 — Analysis of initial energy transfer mechanism and temperature change explanation formative assessment task from Spring 2014

In addition to the low prevalence of collisions or interactions between the solvent and an intact solute, only 31% of analyzed responses referenced formation of interactions between the solvent and dissociated solute (as indicated by the green bar above).

Because so few students included the formation of interactions in their explanations, we wanted to compare students' use of interactions in their explanations to use in representations. Because the coding schemes for explanations and representations were not organized in the same way, a derivative coding scheme was created, as shown in Table 6.4 to allow direct comparison of use of interactions between explanations and representations. The four mechanistic explanation codes and six representation codes were each collapsed into a common set of three codes. The new set of three codes describes use of solute-solvent interactions in either explanations or representations as (*i*) between the solvent and intact solute [*Intact*], (*ii*) between the solvent and solute after it has dissociated or separated [*nonIntact*], or (*iii*) absent [*None*].

Table 6.4 — Common collapsed codes created to allow comparison of student responses to explanation and drawing tasks

<table>
<tr><th>Collapsed Code</th><th>Applicable Explanation Code</th><th>Applicable Representation Code</th></tr>
<tr><td rowspan="2">Intact</td><td>Present-Explicit</td><td rowspan="2">Complete Interactions</td></tr>
<tr><td>Present-nonSpecific</td></tr>
<tr><td rowspan="2">nonIntact</td><td rowspan="2">Absent-nonIntact</td><td>Incomplete Interactions</td></tr>
<tr><td>Some Interactions</td></tr>
<tr><td rowspan="3">None</td><td rowspan="3">None</td><td>No Solute-Solvent Interactions</td></tr>
<tr><td>No Interactions</td></tr>
<tr><td>Off Task</td></tr>
</table>

Using these collapsed codes allows for comparison of the distribution of codes observed in drawing (see Figure 5.7 in Chapter 5) and explanation tasks. Because of the low prevalence of solvent-intact solute interaction codes (Chi-square expected counts less than 5 for both *Intact* codes), Fisher's exact test was used to test for an association between assessment task and students' use of interactions. As shown in Table 6.5, results of a two-sided Fisher's exact test (Fisher test statistic = 2.626, p = 0.292) indicate no association between the type of assessment (explanation or representation) and use of interaction in students' responses. Based on this result, we conclude that while very few students used the formation of interactions between the solvent and any solute as a mechanistic entity to explain the temperature change, they performed no differently on the explanation task than on the representation task.

Table 6.5 — Summary of types of interactions observed in student explanations and drawings of the solvation process in formative assessment tasks from Spring 2014

Solvent-Solute Interactions Present (Collapsed Code)	Explanations (Figure 6.3)	Drawings (Figure 5.7)	Statistics	
Intact	2.9%	4.3%	Fisher's exact test	2.626
nonIntact	31%	19%		
None	66%	77%	*p*-value	0.292

As previously mentioned, there were two separate revisions to the TESA. The TESAv1 separated representation and explanation tasks, instructed students to describe (rather than draw) the energy transfer mechanism present in solvation, and then use the mechanism to explain the observed temperature change. The TESAfinal sought to help students identify relevant explanation components by breaking the prompt into smaller pieces. Students were asked to describe the representation they had previously drawn of the solvation process, explain how energy is transferred, and explain why the temperature of the solution decreased. The initial, first revised, and final revised explanation prompts (and their development) were previously discussed in Chapter 4; the revised versions of the TESA can be seen in Figure 4.14. All three versions of the explanation prompt have been reproduced below for convenience:

Table 6.6 — Summary of explanation prompts developed for formative assessment tasks

Initial	Now draw a picture showing how the energy is transferred between the system and surroundings. Indicate what you are considering the system and what is the surroundings. In the black box explain why the temperature goes down (in the surroundings).
TESAv1	On the previous slide you showed how the dissolving process occurs, at the molecular level. In the black box, describe the molecular level mechanism by which energy is transferred, and use it to explain why the temperature goes down (in the surrounding).
TESAfinal	- Referring to your diagram on the previous slide, **describe** the sequence of events that happens when NaCl dissolves in water.
	- How is energy transferred between the system and the surroundings during this process?
	- When NaCl dissolves, the temperature of the solution decreases. Explain **why the temperature goes down** (in the surroundings).

Students' responses to both revised assessments were analyzed for Fall 2015 (TESAv1) and Spring 2017 (TESAfinal) semesters; results are shown below in Figure 6.4, which includes data from the initial assessment previously shown for comparison. Again, note that "Absent" and "Present" categories on the *x*-axis refer to the absence or presence of interactions between the solvent and the intact solute.

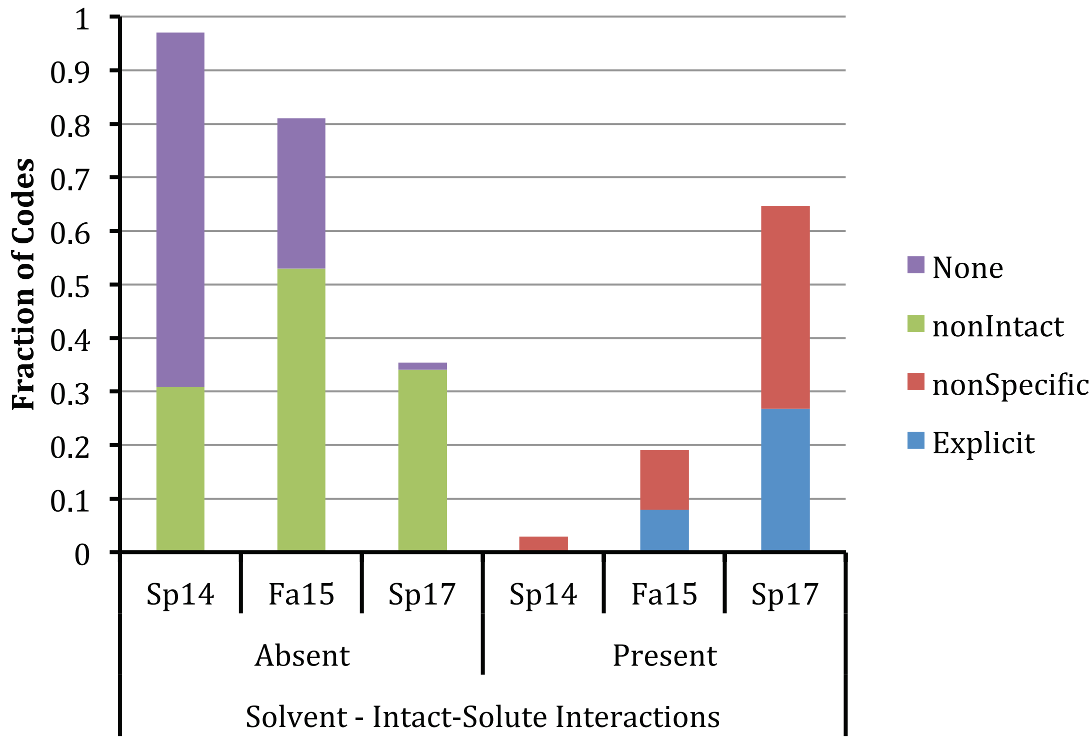


Figure 6.4 — Analysis of interactions used in student responses to initial (Sp14), TESAv1 (Fa15), and TESAfinal (Sp17) *explanation* prompts

More students used the formation of interactions between the solvent and the solute in their explanation of the temperature change accompanying solvation on the TESAfinal than on the TESAv1. Responses to both revised assessments used more interactions than the initial prompt. Chi-square analysis was performed to determine if there was an association between the assessment and use of interactions for these three assessments. Summary statistics are shown below in Table 6.7; complete results are located in Table H.1 in Appendix H.

Table 6.7 — Chi-square statistics testing for association between explanation assessment (initial, TESAv1, or TESAfinal) and students' use of interactions

Chi-Square Test			
	Value	df	Asymptotic Significance (2-sided)
Pearson Chi-Square	113.629[a]	6	<.0005
N of Valid Cases	250		
Cramer's V	0.477		<.0005

The null hypothesis of the test was that there is no association between distribution of codes describing students' use of interactions and the assessment version. Based on results of the chi-square test (χ^2 = 113.629, df = 6, p < 0.0005) we reject the null hypothesis and conclude that there is an association between use of interactions and the assessment version. The Cramer's V obtained from this test (0.477) indicates a medium to strong association between assessment type and the distribution of codes describing students' use of interactions in their explanations. Standardized residuals shown in Table 6.8 were generated to determine which cells are most influencing the statistical difference, and the large effect size, observed in distribution of codes. Positive residuals indicate categories with larger than expected frequency, while negative residuals indicate categories with smaller than expected frequencies. From these results, we can conclude that responses to the initial prompt that did not use any formed interactions contributed the most the observed association (standardized residual of 5.544), followed by responses containing no interactions and those containing nonspecific interactions between the solvent and the intact solute observed on the TESAfinal (standardized residuals of -4.724 and 4.361 for "none" and "nonspecific" responses, respectively). Other contributors to the statistically significant association, including both "present" codes on the initial prompt (low occurence) and the "present-explicit" code for the TESAfinal (high occurrence), are indicated by the "1" superscript, and are themselves significant at the α = 0.01 level (the critical value for the a standardized residual at the α = 0.01 level is 2.58).

Table 6.8 — Crosstabs analysis, including residuals, describing categories contributing to statistically significant association between assessment type and students' use of interactions

Effect of Assessment Version on Interaction Coding						
			Assessment Version			
			Initial Prompt	First Revised TESA	Final Revised TESA	Total
Interaction Code	Present - Explicit	Count	0_a	8_a	22_b	30
		Standardized Residual	-2.857[1]	-1.155	3.876[1]	
		% within Assessment	0.0%	8.0%	26.8%	
	Present - nonSpecific	Count	2_a	11_a	31_b	44
		Standardized Residual	-2.881[1]	-1.573	4.361[1]	
		% within Assessment	2.9%	11.0%	37.8%	
	Absent - nonIntact	Count	21_a	53_b	28_a	102
		Standardized Residual	-1.280	1.910	-.943	
		% within Assessment	30.9%	53.0%	34.1%	
	Absent - None	Count	45_a	28_b	1_c	74
		Standardized Residual	5.544[1]	-.294	-4.724[1]	
		% within Assessment	66.2%	28.0%	1.2%	
Total		Count	68	100	82	250

Each subscript letter denotes a subset of Assessment Version categories whose column proportions do not differ significantly from each other at the α = 0.05 level.
1. Significant contributor to association between task and students' use of interactions at the α = 0.01 level (critical value = 2.58).

In addition to determining major contributors to the association between assessment version and use of interactions, column proportions were compared for each code using a Bonferroni corrected z-test. The Bonferroni methods controls for Type I error ("false" significance) in repeated pairwise comparisons by dividing the α level by the number of comparisons. For each interaction code (row) in Table 6.8, significantly difference proportions are signified by different subscript letters. For example, comparing the initial prompt to the TESAv1, *Present-Explicit* and *Present-nonSpecific* codes do not differ significantly while *Absent-nonIntact* and *Absent-None* codes do differ significantly at the $\alpha = 0.05$ level (Bonferroni corrected). From the data in Table 6.8 we observe that students are able to explain the temperature change and energy transfer mechanism by using the formation of interactions between the solvent and the intact-solute more frequently on the TESAfinal than on either the initial or TESAv1 (see the *Present-Specific* and *Present-nonSpecific* rows in Table 6.8 above). Additionally, each revision (both from initial to TESAv1 and from TESAv1 to TESAfinal) resulted in a significantly lower proportion of responses not containing any interaction formation or collisions.

As of the TESAfinal, over 60% of explanations used the formation of interactions between the solvent and an intact solute to explain the temperature change. This compares favorably to student use of interactions in representing the process of solution formation in the SRA. Recall from Chapter 5 that representations of solution formation that included complete interactions composed approximately 20% of all student responses on formative assessment tasks (see the left panel of Figure 5.8). This finding further supports the need to ask students to produce representations of their understanding *in addition to* constructing explanations of phenomena to provide the most convincing evidence of student understanding.

RQ2: What aspects of the task prompt are effective at eliciting evidence of student understanding?

Statistical tests can provide insight into what types of student responses influenced the association observed above between assessment and interaction use. Unfortunately, it is more difficult to determine *what* caused the increase in interaction use from the initial prompt to the final revised version of the TESA. While the "gold standard" of a randomized treatment-control experiment has the potential the directly identify causal relationships, these are vanishingly rare and difficult to enact, particularly in authentic learning environments (Cooper & Stowe, 2018).

One strategy to attempt to elucidate factors leading to this change is to further investigate the relationship between students' use of interactions in representing the solvation process and in explaining the temperature change that accompanies it. By using a common scale to describe students' use of interactions on both tasks (as was done earlier for the initial prompt; see Table 6.4, Table 6.5, and the surrounding discussion) it is possible to directly compare how students respond to both representation and explanation tasks.

Because treatment of interactions increases from absent to incorporating an intact solute as the collapsed code progresses from *None* to *nonIntact* to *Intact* (again, see Table 6.4 for the set of "collapsed" codes that will be used throughout this discussion), these codes can reasonably be treated as ordinal in nature. That is, more sophisticated treatment of the interactions forming during the solvation process, such as those between the solvent and an intact solute, can be "ranked" higher than less sophisticated, or absent, interactions. This allows for an ensemble test that compares each student's use of interactions between explanation and representation tasks, such as a Wilcoxon Signed Ranks Test (WSRT). The WSRT ranks the changes between two observations (or codes describing use of interactions in this case) *of the same student*, compiles these differences for a population of students, and calculates a test statistic that can be used to characterize whether overall performance increases, decreases, or does not change (Agresti, 2002).

The WSRT results shown below in Table 6.9 compare students' use of interactions in drawing and explanation tasks in the initial prompt from Spring 2014. In this case, negative ranks mean that a student used more sophisticated interactions on the *drawing* task than on the explanation task. Positive ranks indicate that interaction use was more sophisticated on the *explanation* task than on the drawing task. Ties indicate that students used similarly sophisticated interactions in both tasks. The test statistic of the WSRT uses the mean rank of whichever case (positive or negative rank) has the smallest *sum* of ranks. That mean rank can then be transformed into the more familiar z-statistic to obtain a p-value for the test. In this case, negative ranks (where negative ranks mean that the student used more sophisticated interactions on the drawing task than the explanation task) have a smaller sum of ranks, so the test statistic used to determine significance is that of the negative ranks. We also note that the mean rank for negative ranks was larger than for positive ranks, implying that students who used more sophisticated interactions on the drawing task improved slightly more (on average) than students who used more sophisticated interactions on the explanation task. However, the larger number of cases where students used more sophisticated interactions on the explanation task than the drawing task resulted in a statistically insignificant (WSRT: $z = -0.905$, $p = 0.421$) small increase in sophistication of interactions on the explanation task.

Table 6.9 — WSRT for student use of interactions on explanation and drawing tasks from Spring 2014

Ranks

		N	Mean Rank	Sum of Ranks
Explanation Interactions - Drawing Interactions	Negative Ranks	9[a]	15.83	142.50
	Positive Ranks	17[b]	12.26	208.50
	Ties	42[c]		
	Total	68		
Test Statistic	z			-0.906
	Exact. Sig. (2-tailed)			0.421

a. Explanation Interactions < Drawing Interactions
b. Explanation Interactions > Drawing Interactions
c. Explanation Interactions = Drawing Interactions
d. Based on negative ranks

While results from the WSRT capture the overall magnitude of change (or lack of change) across all students' individual use of interactions between the two tasks, it does not consider cases were the type of interactions used did not change. Therefore, this test cannot distinguish between groups solely on the basis of consistently more or less sophisticated usage of interactions across the prompts. In other words, groups containing many low-level ties (where many students consistently use less sophisticated mechanistic ideas about the formation of interactions) are indistinguishable from those containing a similar number of high-level ties (where more sophisticated treatments of interactions are used in both drawing and explanation tasks) before the positive and negative rank cases are accounted for. One way to visualize these data that does not minimize these ties is a Sankey diagram. These diagrams indicate flow between nodes (assessment tasks in the current case) with path widths proportional to the quantity or frequency of that path. The Sankey diagram in Figure 6.5 below graphically displays how students' representation and explanation responses were coded and how they changed (or stayed the same) between the two tasks in the initial assessment from Spring 2014. Interpretation of Sankey diagrams will use the shorthand *Drawing Code* → *Explanation Code* to refer to matched representation and explanation codes. For instance, we can see from the top of Figure 6.5 that the most prevalent single connection is the *None* → *None* tie.

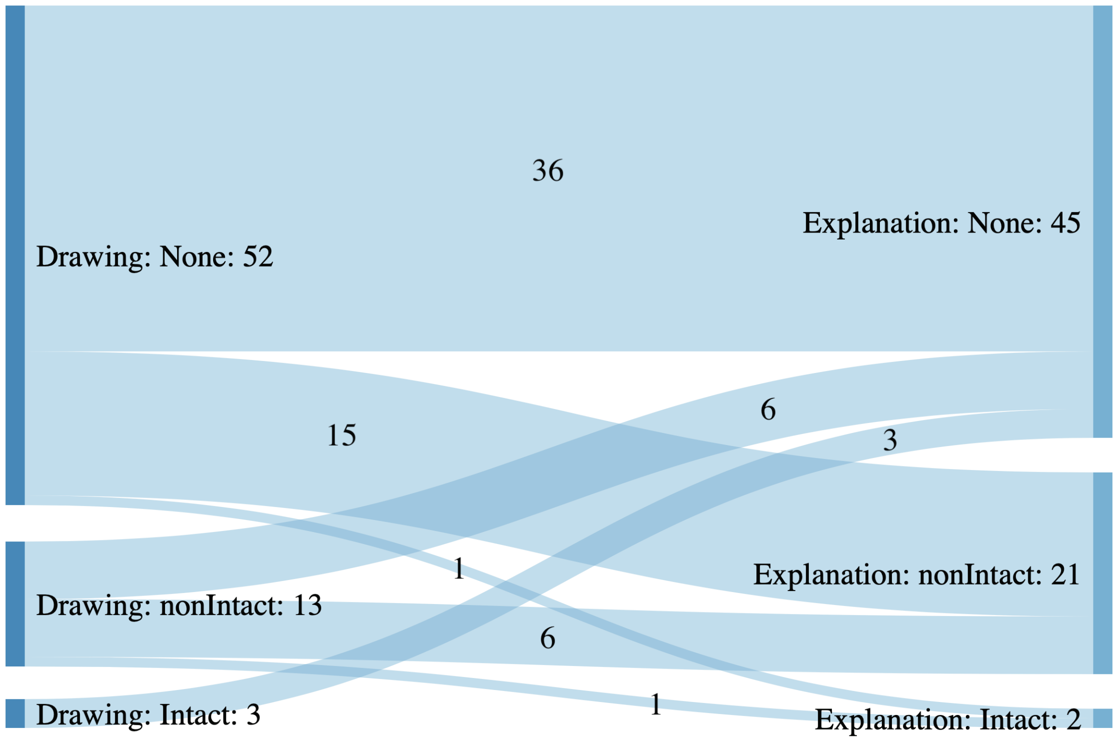


Figure 6.5 — Sankey diagram displaying relationship between students' use of interactions in drawing and explanation formative assessment tasks on the initial formative assessment activity in Spring 2014

From the Sankey diagram it is clear that the majority of ties resulted from representations and explanations that did not include the formation of interactions between the solvent and the solute (intact or otherwise). In fact, 36 of the 42 ties did not include interactions between the solvent and a solute at all, and were therefore coded as *None*. Additionally, no student in the sample both represented and explained the solvation process as containing interactions between the solvent and an intact solute. More interestingly, all three students who represented the solvation process as containing interactions between the solvent and the intact solute explained the temperature change without discussing the formation of interactions between the solvent and solvent or collisions of any variety. The results seen in this section suggest that, like the representation task described in Chapter 5, the initial explanation prompt largely did not support students' construction of explanations that utilized the formation of interactions as mechanistic elements.

A similar analysis, consisting of constructing relevant Sankey diagrams and performing and interpreting WSRT, was performed for results of the TESAv1 in Fall 2015 and the TESAfinal in Spring 2017. Beginning with the Sankey diagram for the TESAv1 from Fall 2015 (see Figure 6.6 below), the most obvious difference is the reduction in *None* → *None* ties accompanied by the emergence of the *Intact* → *Intact* tie at the bottom of the figure. Additionally, the Fall 2015 Sankey diagram is qualitatively much more symmetrical than the "top-heavy" diagram in Figure 6.5 which represented the high frequency of less sophisticated use of interactions in both representation and explanation tasks in Spring 2014.

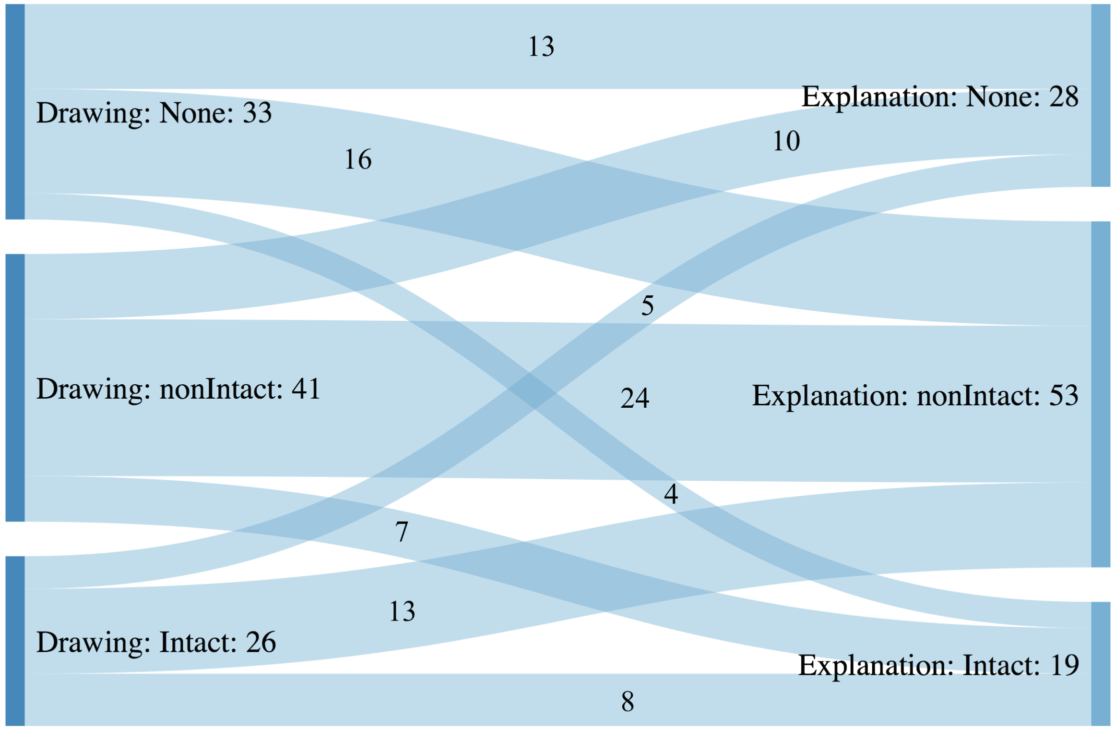


Figure 6.6 — Sankey diagram displaying relationship between students' use of interactions in drawing and explanation formative assessment tasks on the TESAv1 in Fall 2015

Chi-square analysis was performed to determine if there was a significant association between task (representation or explanation) and students' use of interactions when using the TESAv1 in Fall 2015. Based on results of the chi-square test (χ^2 = 3.031, df = 2, p = 0.220) there is no statistically significant association between students' use of interactions and the assessment task (see Table H.2 in Appendix H for further details).

Although there is no association between distribution of codes and assessment type, a WSRT was performed to assess whether students performed differently on the two tasks. These results also indicate no difference in student's use of interactions from drawing to explanation tasks (z = -0.231, p = 0.841). As suggested by the symmetry observed in the

Sankey diagram above, negative (28 cases) and positive (27 cases) ranks were nearly equally prevalent. For further details see Table H.3 in Appendix H.

Recall that results from the TESAv1 contained significantly fewer *Absent-none* codes and significantly more *Absent-nonIntact* codes than the initial assessment in Spring 2014 (see Table 6.8). The current finding, that there is no difference in students' use of interactions in representation and explanation tasks, implies that there is nothing in this version of the assessment that preferentially supports students to use more sophisticated ideas about the formation of solute-solvent interactions and/or collisions when explaining the temperature change that accompanies solution formation.

With this in mind, attention turns to student responses to the TESAfinal, administered in Spring 2017. The codes observed in student responses and chi-square statistics are shown below in Table 6.10. The calculated chi-square statistic (χ^2 = 38.051, df = 2, p < 0.0005) indicates that there is a significant association between the assessment type (drawing or explanation) and students' use of interactions. The Cramer's V of 0.482 indicates a medium to strong association between assessment type and use of interactions. Analysis of standardized residuals indicates that differences in the *None* code (relative presence in drawings and relative absence in explanations) is the largest factor contributing to the observed association (and is a significant contributor to association at the α = 0.01 level). Students' use of intact-solute interactions was a secondary factor contributing to the association, and was significant at the α = 0.05 level.

Table 6.10 — Chi-square statistics testing for association between assessment type and student's use of interactions in the TESAfinal, Spring 2017

			Task		Total
			Drawing	Explanation	
Interaction Code	Intact	Count	24_a	53_b	77
		% within Task	29.3%	64.6%	47.0%
		Standardized Residual	-2.3[2]	2.3[2]	
	nonIntact	Count	28_a	28_a	56
		% within Task	34.1%	34.1%	34.1%
		Standardized Residual	.0	.0	
	None	Count	30_a	1_b	31
		% within Task	36.6%	1.2%	18.9%
		Standardized Residual	3.7[1]	-3.7[1]	
Total		Count	82	82	164
		% within Task	100.0%	100.0%	100.0%

	Value	*df*	Asymptotic Sig (2-sided)	Exact Sig. (2-sided)	Cramer's V
Pearson Chi-Square	38.051	2	<0.0005	<0.0005	0.482

Each subscript letter denotes a subset of Task categories whose column proportions do not differ significantly from each other at the .05 level.
1. Significant contributor to association between task and students' use of interactions at the $\alpha = 0.01$ level.
2. Significant contributor to association between task and students' use of interactions at the $\alpha = 0.05$ level.

We additionally observe the statistically significant differences (Bonferroni corrected z-test) at the $\alpha = 0.05$ level in proportion of *Intact* and *None* codes observed in representation and explanation responses. *Intact* responses were approximately twice as likely to be observed in explanations, while *None* responses were virtually absent in explanations. These results, the larger proportion of more sophisticated use of interactions in explanations than in drawings and higher occurrence of representations without interactions between the solute and the solvent, imply that students used more sophisticated treatments of interaction formation on explanation tasks than in drawings.

A WSRT was performed to formally measure if students used more sophisticated interactions in drawing or explanation tasks. The resulting test statistic

(z = -5.938; $p < 0.0005$) indicates that there is a significant difference in students' use of interactions in the two assessment types. Because the test statistic is based on the smaller mean rank, the effect size (-0.461) indicates a medium to large *negative* effect for negative cases, meaning that negative cases are much less likely and therefore more sophisticated use of interactions was observed in explanations than in drawings. Summary statistics are shown below in Table 6.11; the data for this analysis are presented graphically in a Sankey diagram in Figure 6.7.

Table 6.11 — WSRT for student use of interactions in drawing and explanation responses to the SRA and TESAfinal in Spring 2017

Ranks

		N	Mean Rank	Sum of Ranks
Explanation Interactions - Drawing Interactions	Negative Ranks	4[a]	20.50	82.00
	Positive Ranks	49[b]	27.53	1349.00
	Ties	29[c]		
	Total	82		
Test Statistic	z		-5.938[d]	
	Exact. Sig. (2-tailed)		<0.0005	
	Exact Sig. (1-tailed)		<0.0005	
	Effect size r		-0.461	

a. Explanation Interactions < Drawing Interactions
b. Explanation Interactions > Drawing Interactions
c. Explanation Interactions = Drawing Interactions
d. Based on positive ranks.

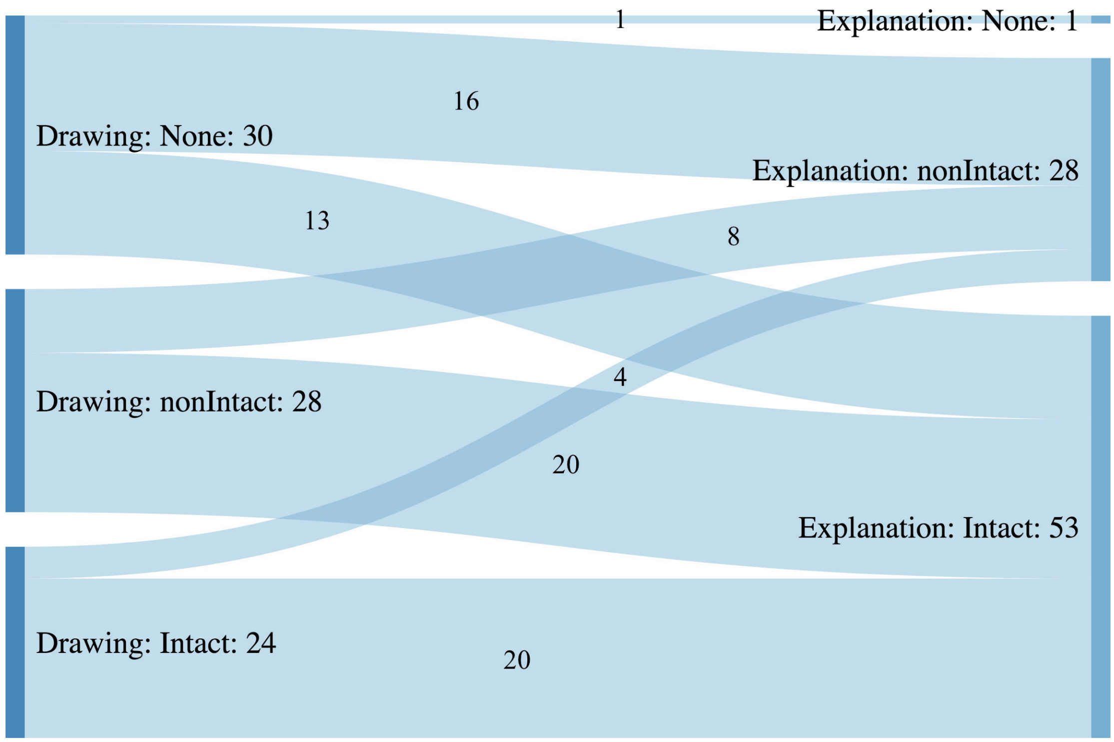


Figure 6.7 — Sankey diagram displaying relationship between students' use of interactions in drawing and explanation formative assessment tasks on the SRA and TESAfinal in Spring 2017

The Sankey diagram showing how students used interactions on drawing and explanation tasks of the SRA and TESAfinal in Spring 2017 supports the results of the chi-square test of association (Table 6.10) and the WSRT (Table 6.11) previously discussed. Indeed, the diagram constructed to characterize results from Spring 2017 looks very different from the diagram displaying results from the initial prompts from Spring 2014 (see Figure 6.5). Here we note the near absence of the *None* → *None* tie (only one occurrence, at the top of the figure), the large number of *Intact* → *Intact* ties, and the presence of just a single pathway resulting in less sophisticated treatment of interactions for explanations than for drawings (*Intact* → *nonIntact*). Furthermore, the vast majority (49 of 82) of cases resulted in positive rank, where explanations used more sophisticated treatment of interactions than in drawings. This is evident by the steady flow of the diagram down and to the right.

Based on the magnitude of these results, both in terms of effect size of the difference and in the virtual absence of explanations with no apparent use of interactions, another sample from a different semester was analyzed to see if these results were replicable. Using the same sample of students from Fall 2016 as in Chapter 5, a significant increase in sophistication of interactions used in explanations was again observed (WSRT: $z = -4.687$; $p < 0.0005$, r = -0.364 for negative cases) *despite* differences ($\chi^2 = 16.205$, $df = 3$, $p = 0.001$, Cramer's V = 0.313) in the distribution of the codes themselves between the two semesters. Summary statistics for the WSRT, Sankey diagram, and full crosstabs analysis for this replication are shown in Table H.4, Figure H.1, and Table H.5, respectively, in Appendix H.

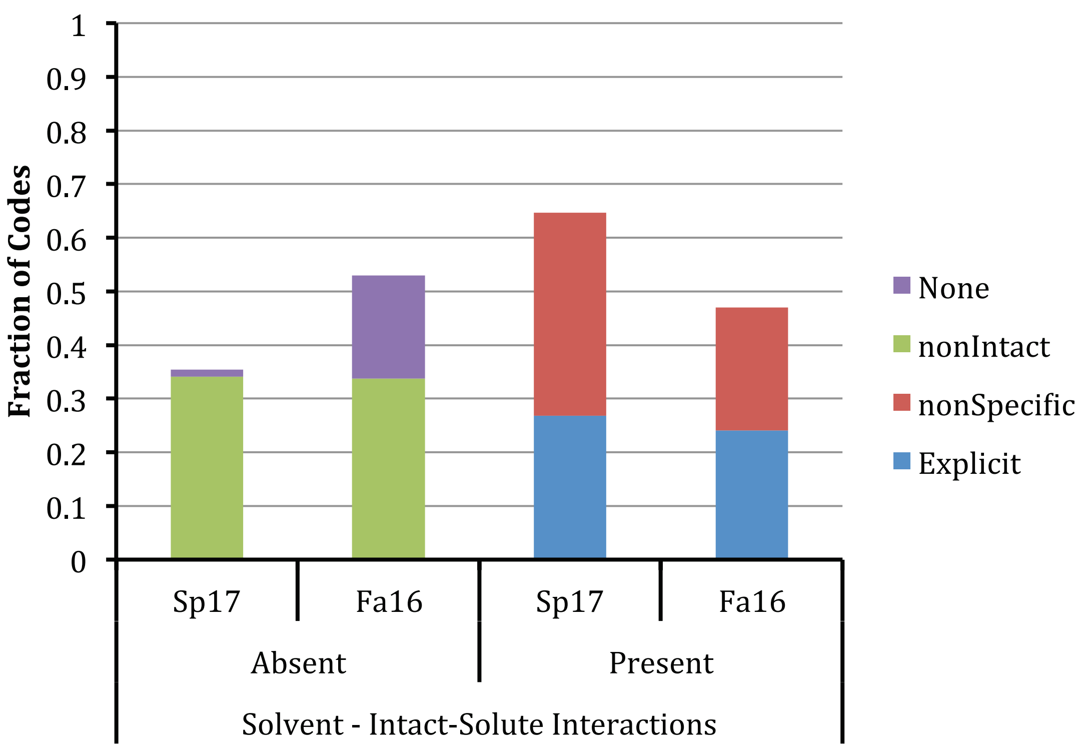


Figure 6.8 — Analysis of interactions used in student responses to final revised (Sp17) and replication (Fa16) explanation prompts

The data in Figure 6.8 show the replication data had a higher fraction of "None" codes and a lower fraction of both "Explicit" and "nonSpecific" codes. Crosstabs analysis (see Table H.5) indicate that the low fraction of "none" responses in the original Spring 2017 analysis was the primary contributor to the difference between the two distributions. This data suggests that the TESAfinal is able to elicit more sophisticated use of interaction in students' explanations than in their representations, both for populations with relatively high overall use of interactions (e.g. Spring 2017) and for populations with somewhat lower overall use of interactions (e.g. Fall 2016).

In addition to how successful students were in using concepts of forming interactions with an intact solute in their explanations, responses to the TESAfinal were the first observed case in the current research that demonstrably showed better performance (more sophisticated use of interactions) than a similar task completed in the same assessment sequence. This prompts the question:

> What is it about the TESAfinal that resulted in such a measurable increase in using interactions in such a way that implies a more mechanistic understanding of the underlying solvation process?

The prompts given to students in the first and final TESA revisions have been discussed at length previously, and are re-presented below for convenience in Table 6.12. By highlighting tasks given to students that are in both prompts we are able to identify the main differences that were made to the final version of the TESA.

Table 6.12 — Summary of TESA prompts; similar tasks are color-coded in both versions, the newly developed instruction is outlined and color-coded grey

TESAv1	On the previous slide you showed how the dissolving process occurs, at the molecular level. In the black box, describe the molecular level mechanism by which energy is transferred, and use it to explain why the temperature goes down (in the surrounding).
TESAfinal	- Referring to your diagram on the previous slide, **describe** the sequence of events that happens when NaCl dissolves in water.
	- How is energy transferred between the system and the surroundings during this process?
	- When NaCl dissolves, the temperature of the solution decreases. Explain **why the temperature goes down** (in the surroundings).

The first difference, that is perhaps most obvious to students, is the structure of the question and response area. The TESAv1 was composed of the prompt seen above (without the color coding) at the top of the slide and a single large response area filling the rest of the slide (as originally shown in Figure 4.11a). The TESAfinal is composed of three smaller instructions or questions, each of which has its own text box (see Figure 4.11b). In this way, the assessment was constructed to scaffold students as they collected the components necessary to construct their explanation of the origin of the given temperature change that accompanied solution formation.

For reasons described below, I suggest that students' success on the TESAfinal was not solely attributable to structural scaffolding provided by explicitly providing separate text boxes in which students could attend to the various components of their nascent understanding of the process and explanation of solution formation (and any accompanying temperature change). Instead, I propose that the primary driver of the observed increase in sophistication of students' use of interactions is the first thing asked of students when they encountered the revised TESA prompt:

"**Describe** the sequence of events that happens when NaCl dissolves in water."

I suggest that this part of the prompt was particularly helpful for three reasons.

First, prompting students to think about and describe in words what happens in order for the solute to dissolve adds an extra step that is relevant to answering the question. By structuring the task such that students were able to start with a *What* explanation before progressing to more complicated *How* and *Why* levels of explanation (Braaten & Windschitl, 2011), the prompt was able to call attention to aspects of the system, and phenomenon, that may have been taken for granted. It has been suggested that this deliberate structuring of the formative assessment task to explicitly call attention to potentially overlooked components is one scaffolding strategy that can support students to construct more sophisticated explanations (Reiser, 2004; Reiser & Tabak, 2014).

In addition to allowing students to begin their explanations with a less complex explanation (the *What* prompt, as described above), this descriptive prompt allows students to slow down their thinking. Research has shown that general chemistry students often employ heuristics to help them respond to comparison or explanation tasks under time pressures. While these strategies can help in limited cases, the use of heuristics often lead students to incorrect conclusions such as one-component reasoning (Boo, 1998; Maeyer & Talanquer, 2010, 2013). This is particularly relevant in chemistry since most heuristics are based on personal experiences of the physical world, which we have previously described as far removed from the unintuitive world of the atomic-molecular scale.

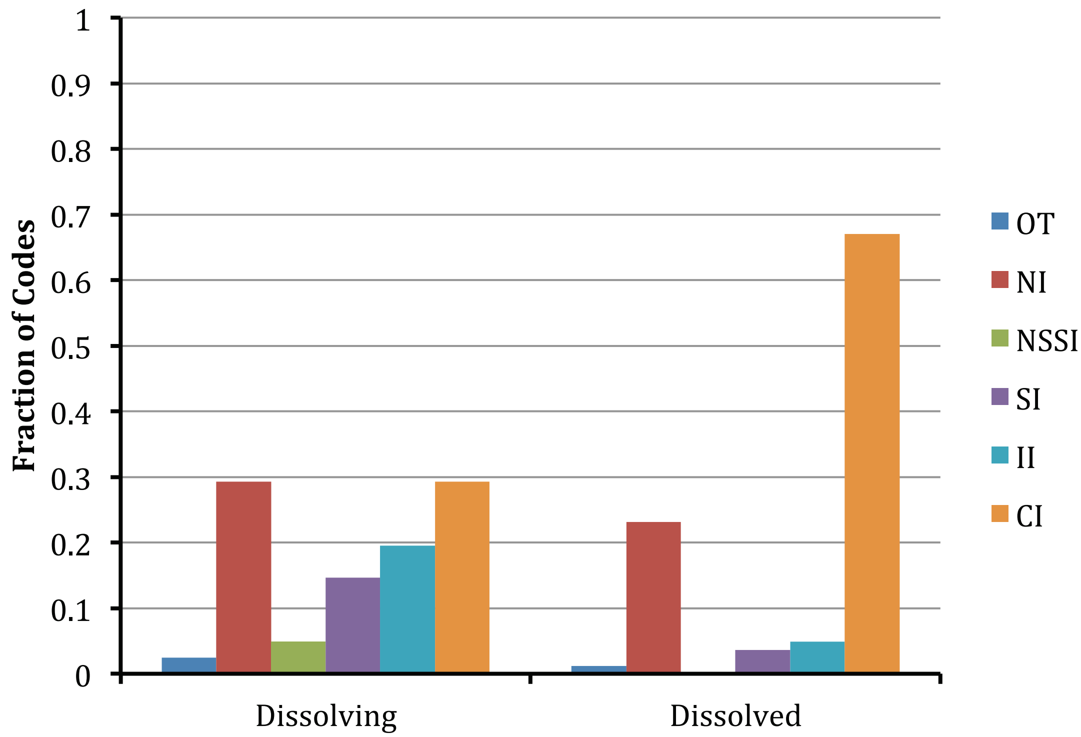


Figure 6.9 — Analysis of SRA responses from Spring 2017 as administered in formative assessment. Code abbreviations in the legend are the same as previously defined in Table 5.2.

A final reason I suggest that it is the *What* prompt that results in most of the difference observed in students' increased use of forming interactions, from drawing to explanation tasks, is the part of the prompt that is not actually asking the student to do anything. The *What* prompt begins with the following language: "Referring to your diagram on the previous slide (use the "Previous" button if needed)". Here we see that the prompt explicitly reminds students that they can go back and look at their work on the previous slide while describing the sequence of events that occurred when sodium chloride dissolved in water. While there is no way to record how students move between slides of an activity (only the timestamp of the most recent submission is recorded in beSocratic), I call attention to Figure 6.9 where we see that over 65% of formative assessment representations of the fully dissolved solution contained complete interactions. Had they gone back, well over half of the students would have seen their representation on the previous slide, complete with interactions between the solvent and the solute. Regardless of when students described these interactions forming, they all would have been coded as *Present* (whether *Intact* or *nonIntact*), which could account for some of the increase observed in students' use of interactions on the explanation task.

While many possible explanations for how the revised scaffolding implemented in the TESAfinal have been suggested, it is ultimately quite difficult to state with confidence what specifically contributed (and by how much) to the observed increased use of interactions on the final revised explanation prompt.

Conclusions and Implications

Previously, this dissertation has described the development of: formative assessments designed to facilitate and support students as they construct their understanding of observable dissolving phenomena to atomic-molecular scale interactions, energy, properties, and changes; assessments intended to elicit students' representational understanding of the solvation process; and methods to evaluate and characterize the interactions students use in those representations as markers of mechanistic understanding.

In this chapter I have discussed the development of a coding scheme to characterize students' mechanistic understanding of the dissolving process by characterizing the use of interactions in explanations of an observable temperature change that accompanies solution formation. By focusing on interactions it is possible to collect evidence about how students are thinking mechanistically about the process by which a simple ionic compound dissolves in water. Thus far, the primary application of this coding scheme has been to evaluate assessment revisions.

The current research has shown that students in the CLUE curriculum are able to use the formation of interactions in explanations of a temperature change observed when solutions form over 80% of the time. Furthermore, students use the formation of interactions between the solvent and an *intact* solute over half of the time, and explicitly refer to the sub-molecular species interacting and removing ions into solutions in approximately a quarter of responses. These results are important because they demonstrate these students' ability to discuss components required to construct causal mechanistic explanations of a complicated chemical phenomenon after limited instruction.

The second central finding in this study is related to how students' use of interactions in explanation tasks changed when the assessment was revised. The increased use of interactions provides further evidence in support of evidence centered assessment design and scaffolding strategies. These results represent the first time that students' ability to produce and use mechanistic components in an explanation of the temperature change that occurs during solution formation has been systematically measured at scale.

The final implication relates more generally to assessment design. We have previously seen that students in the CLUE general chemistry curriculum are able to successfully represent aqueous ionic solutions as being composed of isolated ions; each interacting attractively with solvent molecules despite extensive published literature documenting student difficulty on these kinds of tasks (see Chapter 5 for more details). One of the findings from analyzing representations of the solvation process was that whole class distributions of codes describing students' use of interactions in summative assessment tasks were not statistically different from each other, regardless of performance on formative assessments. From this we concluded that differences observed in students' ability to represent the interactions present *during* solvation could be attributed to changes in the format of the assessment task itself. An important extension of this finding, which has also been observed in the current study analyzing students' use of interactions in explanations, is that absence of evidence (for instance absence of interactions in an explanation) is not evidence that understanding is absent. More specifically, we have observed that as the explanation assessment was revised from an initial task to the final revised TESA that the fraction of students not including *any* discussion of interactions decreased from over 60% to approximately 10%. Over this same time, students' use of explicit descriptions of submolecular species participating in the formation of interactions (which was not observed at all in responses to the initial assessment) increased to just over 20%.

This finding highlights the importance of carefully designing free-response assessments to elicit student understanding, especially when there are multiple levels (macroscopic, symbolic, molecular, or subatomic) at which a phenomenon could be explained or described. Whereas other methods of assessment (e.g. multiple choice or interview) can clearly define or elicit further elaboration of student understanding (e.g. by changing the wording of multiple choice options or further prompting for student thinking in an interview setting) the constructed response format only has one opportunity to elicit a student's response. It is crucial that assessment prompts are designed to elicit student responses at a level that can actually provide *evidence* of their knowledge before making *claims* about their understanding (Mislevy & Haertel, 2006; Mislevy, Steinberg, & Almond, 2003).

Put more plainly: just because a student does not say something does not mean that she does not know it. It may simply mean that she did not interpret the prompt as requiring any further elaboration. An additional aspect of these findings is that they provide a way of thinking about student performance that moves away from deficit models of student knowledge. By designing assessments in ways that are deliberately intended to support students in using their knowledge, especially by helping them activate resources relevant to demonstrate their understanding (Hammer & Elby, 2003), we can communicate the purpose of assessment as one of supporting students' expression of understanding, rather than that of extracting knowledge.

Limitations and Future Work

The limitations present in the current analysis of students' explanations of the temperature change that accompanies solution formation closely mirror those of the previous analysis of students' representations. This work has only looked at how CLUE general chemistry students, at a single university, use ideas of interaction formation in their explanations. It will be important for future research to study if and how interaction use in these explanations varies for different student populations and learning environments as CLUE experiences further adoption (and adaption, in the case of implementation in secondary schools).

The second limitation is related to the specificity with which the research question was developed. Because I have chosen to focus so closely on how students' explanations provide evidence that they understand or are thinking mechanistically about the solvation process, use of interactions was prioritized over entropic and enthalpic contributions. Additionally, because responses to formative assessment items were analyzed in this work, very little emphasis was placed on the "correctness" of explanation components. This conscious decision was made so that anticipated difficulties students might have had, perhaps related to the energetics of breaking and forming interactions, did not overwhelm the productive ways that interactions were used in their explanations. A logical extension of this work would likely integrate students' conceptions of energetic and enthalpic contributions to the solvation process in general, and the observed temperature change in particular. I point out that inclusion of students' understanding and use of entropic contributions to the solvation process would likely require further development of the assessment, since very few students included these ideas in their explanations of the observed temperature change.

The final suggestions for further development of this research concern development of the TESA. One unanswered question is related to what aspects of the revision actually contributed to the observed increase in use of interactions. A strategy to further investigate the individual effects of scaffolding features could involve administering different versions of the TESA (perhaps only using different response areas or only using the *What*, *How*, *Why* prompting) to different groups of students. Before continuing, I think it important to note that it is entirely likely that the revisions resulted in increased use of interactions *because* they were used simultaneously. In other words, the interaction of the two scaffolding strategies might be larger than the sum of their individual usage (which would, in and of itself, be an interesting result if it could be replicated).

Finally, recalling the discussion of the principles of scaffolding enacted in the development of the final revised version of the TESA, one of the principles of scaffolding that is not often enacted is that of fading. When fading is implemented, aspects of the scaffolding are gradually removed over time as the learner gains expertise, with the expectation that she will ultimately be able to complete the task without the previously provided support (Sherin et al., 2004). Future work to study how students' use of mechanistic components (the formation of interactions) in explanations is maintained over time could introduce fading by first removing the separate response areas (and maintaining the *What*, *How*, *Why* structure) before implementing an unscaffolded prompt.

CHAPTER 7 — CONCLUSIONS, IMPLICATIONS, AND FUTURE WORK

The research reported in this dissertation has been concerned with assessing and characterizing students' understanding of solutions and the process of solvation. While there are many factors that must be taken into account to provide a complete description of this process, I have focused my work on describing how responses to these representation and explanation prompts provide evidence that students' have a *mechanistic* understanding of what is happening during solvation. This is, how do students' constructed drawings and explanations indicate that they understand what is happening at the atomic-molecular and subatomic-molecular levels?

Conclusions

Students' representation of solutions and the solvation process

In Chapter 5 I described analysis of how students used interactions in their representations of both fully and partially dissolved aqueous solutions of ionic salts. As stated previously, there are extensive reports in the literature documenting student difficulty representing solutions as being composed of separated solute ions individually solvated by solvent molecules (Abell & Bretz, 2018; Ebenezer, 2001; Herrington et al., 2017; Kelly & Jones, 2007, 2008; K. C. Smith & Nakhleh, 2011; K. J. Smith & Metz, 1996).

Despite this anticipated difficulty, students in the CLUE general chemistry course performed very well representing dissolved solutions appropriately. In the current work, 58% of representations produced in formative assessment settings (assigned for homework after one of two lectures covering aqueous ionic solutions) and 87% of representations produced in summative assessment settings contained complete interactions of separated ions interacting appropriately with water molecules. Considering the work of Kelly and Jones (2007) provides a case for comparison. In their work, they observed 14 of 18 (~78%) of students represent dissolved solutions as being composed of solvated ions immediately after viewing particulate level animations of the solvation process. However, in a follow-up study one week later, they observed that none of the same students represented aqueous sodium chloride as containing solvated ion when in a new context (i.e. as a reactant in a precipitation reaction) (Kelly & Jones, 2008). Students in this research were similarly successful representing dissolved solutions as including hydration sphere interactions on an exam assessment approximately a week after the formative assessment as the students in a much smaller (and purposefully sampled) study were directly after viewing particulate level animations (Kelly & Jones, 2007).

When considering the results of students' use of interaction in representing the solvation process (the central "dissolving" panel of the SRA) there is a much less robust literature base against which to compare the current results. While there are numerous reports of difficulties students have in representing dissolved solutions and undissolved ionic salts, very little of the literature has noted how students think about the process by which a solute dissolves (e.g. Abell & Bretz, 2018; K. C. Smith & Nakhleh, 2011) and even fewer have reported results of a study where this was a primary interest. With these considerations in mind, once again I turn to the work of Kelly and Jones (2007) to provide context for the current results regarding students' use of interactions in representing the dissolving process. In their work, 7 of 18 (~39%) of students drew or wrote about solvent molecules pulling ions apart from an intact solute immediately after viewing particulate level animations of the solvation process. While it was not the focus of their follow-up study, 5 (of 18, ~28%) students mentioned the interaction of solvent molecules pulling ions from the lattice to dissolve sodium chloride as a component of dissolving one week later (Kelly & Jones, 2008).

In the current research, 21% of formative assessment representations and 43% of summative assessment representations of the solvation process (in responses to the SRA) contained interactions between the solvent and an intact solute. Students in the CLUE general chemistry course produced representations of the solvation process including interactions between the solvent and an intact solute at roughly the same rate on a midterm exam (approximately a week after the formative assessment activity) as Kelly and Jones (2007) observed for students directly after viewing particulate level animations of the solvation process. Additionally, students who included an intact solute in their representation of the solvation process were two to three times more likely to also include interactions between the solvent and that intact solute. I suggest that finding a way to further support students to consider the requirements of solvation, particularly that there must be an intact solute present, could facilitate construction of representations that include all appropriate structures and interactions.

<u>Students' explanation of macroscopic energy changes that occur during solvation</u>

In Chapter 6 I discussed analysis and development of an assessment prompt asking students to explain an observed macroscopic temperature change that occurs when a solution forms. The key aspect of this explanation that formed the basis for characterizing student responses is, once again, how students included ideas related to formation of interactions between the solvent and the solute. By focusing on these interactions it was possible to compare how students used mechanistic ideas in their representations and their explanations.

This research has shown that CLUE students responding to the TESAfinal were successfully able to include the idea that interactions must form between the solvent and the *intact* solute in their explanations over half of the time. Furthermore, students explicitly identified the submolecular entities (in the solvent) that would individually interact with solute ions to cause the solution to form approximately 25% of the time. A final ~30% of explanations referred generally to the formation of interactions while explaining the temperature change. Overall, over 80% of responses to the final revised assessment used the formation of interactions between the solute and the solvent. We do still observe examples of what Maeyer and Talanquer (2010) refer to as *one-reason decision making*, as indicated by explanations that only referred to overcoming interactions.

To my knowledge, this is the first large scale study characterizing how students use interactions to describe solution formation, so there is little opportunity for explicit comparison to previous work beyond anecdotal observations of similar reasoning across studies such as: collisions supplying energy to overcome ionic bonding (K. C. Smith & Nakhleh, 2011); formation of interactions between the intact solute and the solvent as necessary to cause dissolving to occur (Abell & Bretz, 2018); and student identification of a single causal driver, like the breaking of interactions causing a process to be endothermic (Maeyer & Talanquer, 2010). However, the results of this research are important because they demonstrate CLUE students' ability to discuss components required to construct causal mechanistic explanations for a complicated chemical phenomenon after limited instruction. It is this last point that suggests that CLUE is capable of addressing calls for "major changes [to be made] in the teaching of chemistry if we want students to learn to think mechanistically" (Talanquer, 2018, p. 1096).

Implications

Student Success in CLUE

Given how successfully CLUE students represented aqueous solutions in both revised and initial prompts, I suggest that the repeated explicit references to connections among molecular structure, interactions, energy, and properties across concepts supports students' ability to depict the molecular-level interactions present in solutions. Previous work in our group has shown that students in the CLUE curriculum are particularly well-equipped to draw and use structures to make predictions about properties (Cooper et al., 2012). Instruction on solutions builds upon this foundation by explicitly drawing on students' understanding of interactions and intermolecular forces to explain why, for instance, ethanol is miscible in water, but not hexane. Because electrostatic and bonding interactions (and particularly intermolecular forces) are used throughout the course, students only need to understand the way(s) in which these familiar concepts are applied to solutions. The success that these students had in this research is further evidence that the structure of the CLUE curriculum, including the frequent explicit linking of new material to prior knowledge, can support student success as they encounter historically difficult content.

Prompt Development

Results from analysis of students' representations and explanations suggest both specific implications for assessment design and a larger overall implication concerning the nature of assessment itself. Both assessments (the SRA for representations and the TESA for explanations) utilized evidence centered design to define what evidence of student understanding might look like (Mislevy, Almond, et al., 2003; Mislevy & Haertel, 2006). Scaffolding was then designed to support students' construction of responses containing this evidence. In practice, revisions implemented scaffolding intended to explicitly call attention to aspects of the phenomenon that might be potentially overlooked (Reiser, 2004; Reiser & Tabak, 2014): the "during" phase of solvation for representations, and the physical process by which solutions were formed (as prompted by the "describe the sequence of events…" prompt) for explanations. Additionally, the TESA final was structured to allow students to begin with more descriptive *What* task before progressing to more sophisticated, and difficult to construct, *How* and *Why* explanations as suggested by Braaten and Windschitl (2011). The increased use of interactions observed after the revised items were administered (in both representations of the solvation process and in explanations of the temperature change) suggests that knowing how student responses will provide evidence of understanding offers a particularly effective lens through which assessment design can be viewed. For my last point related to specific details of assessment development, I note that the presence of deliberate scaffolding on the SRA and TESA did not reduce these tasks to trivial exercises. That is, the presence of new scaffolding did not immediately result students being uniformly successful on these tasks. I specifically mention this to make an important argument: a properly scaffolded assessment does not simply *give* students the answer (Berland et al., 2016; Krist et al., 2018), it instead supports student success by facilitating (or removing) aspects of the task that are not currently accessible to the student (Collins, Brown, & Newman, 1989).

The final point I want to make here relates holistically to how assessments are developed and how students' responses are interpreted. Based on the findings of the current work, it is imperative that assessment prompts be structured in such a way that is meaningful to students to elicit responses at an appropriate level of detail to provide evidence of mechanistic understanding. Inherent in the call to structure assessment prompts in a way that is meaningful to students is the need to disaggregate the things we want students to do so that reading the mind of the assessment designer is not the most important aspect of the task. By designing tasks that are clear in their expectations, we can increase the likelihood that students' responses will reflect what they know and can do, rather than just what they thought was the most appropriate way to respond to a potentially ambiguous, unclear, or confusing prompt. As educators and education researchers, we accept that we can never fully know what students know, but we attempt to elicit evidence of what they know through well-structured assessments. This leads to an unavoidable conclusion: just because a student does not perform on an assessment does not mean that she *cannot* perform. It might merely mean that the task did not adequately signal to her what specific performances would demonstrate understanding or mastery.

Future Work

This research provides many avenues for further study, both by direct extension and by using the current results as starting points.

One of the most straightforward areas for future work would be investigating how different populations perform on these same assessment tasks. This work would likely seek to characterize students in different implementations of the CLUE curriculum (to provide evidence about the adaptability of the curriculum itself), including populations from different types of institutions and those with different demographic makeups. It would also be interesting to test these assessments in different curricula to investigate if and how the range and distributions of responses change.

One of the consequences of deciding to focus so closely on characterizing evidence of students' mechanistic understanding was that the coding schemes that were developed do not generally attempt to capture aspects of student responses that do not contribute to "how" or "why" the solvation process occurs. Additional research relating students' use of interactions to entropic and/or enthalpic components could provide insight into the ways students understand solutions and solvation (specifically), and (more generally) the relationship between observable phenomena at the macroscopic scale and interactions, energy, structure, and properties at the atomic-molecular level. Incorporating students' use of entropy could be very interesting here, since endothermic dissolving processes are one of the few phenomena typically encountered in general chemistry that are entropically driven.

Observations of how student responses changed as assessments were revised suggest that further study of the individual and combined effects of components of assessment revision on student responses could be fruitful. It would be interesting to see if certain scaffolding components were more or less effective than others, or if some scaffolding components are only effective when used as part of a larger scaffolding strategy. A final possibility (with respect to studying the effect of scaffolding) would be to systematically fade the supports provided in these assessments. While this research could demonstrate whether students' understanding of solutions and solvation is durable, perhaps a more interesting result could characterize if these prompts were able to scaffold students' use of the *Practices* themselves.

Another way this research could be extended might be to substantially change the system. For example, such work might consider solutions and solvation for polar molecular (not ionic) solutes. An activity was recently designed using a similar format as the current one, but instead prompting students to represent and explain ice dissolving in cold ethanol. In addition to addressing a dissolving phenomena that does not require complete "dissociation" of the solute (compared to the ionic bonding interactions in sodium chloride), this system could also prompt student thinking related to another widely documented difficulty: that students often confuse dissolving and melting processes. Theoretically these tasks (water dissolving in ethanol) are asking very similar questions to those analyzed in this dissertation. However, I would assume that the familiarity of dissolving salt in water (in everyday life) as compared to how unfamiliar it must be to consider water dissolving in ethanol would result in the presence of many different, and likely disconnected, ideas in students' responses.

A final avenue for future work might consider another setting in which a macroscopic temperature change could be described and understood by considering the atomic-molecular level structure, properties, interactions, and energy changes: simple chemical reactions. It would be interesting to find out if and how students' understanding of the atomic-molecular origin of macroscopic temperature changes involved in solution formation informs (or is similar to) their understanding of the atomic-molecular origin of macroscopic temperature changes that accompany, for instance, a combustion reaction.

APPENDICES

APPENDIX A — ORIGINAL FORMATIVE ASSESSMENT ACTIVITY

Initial data collection utilized a formative assessment activity developed for the CLUE curriculum prior to the current research. This activity is presented here in full as it would have been viewed and completed by students in the beSocratic environment.

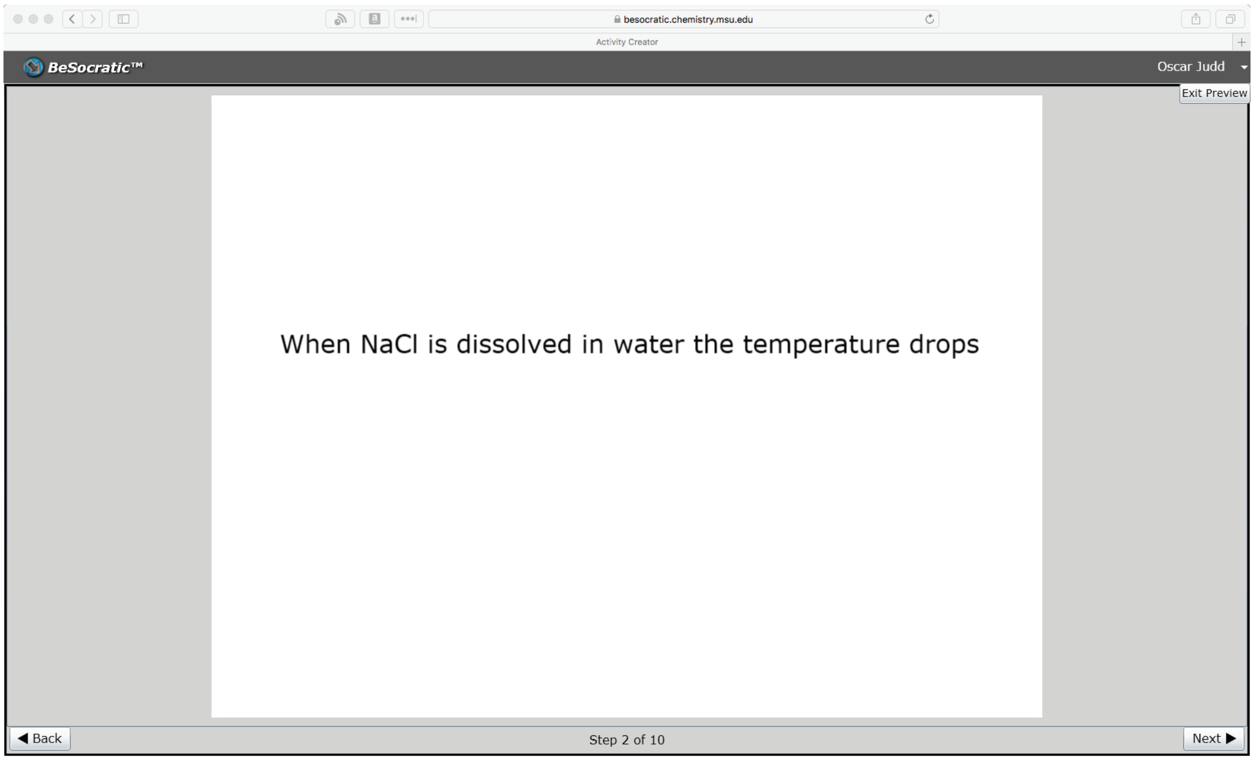


Figure A.1 — Introduction slide

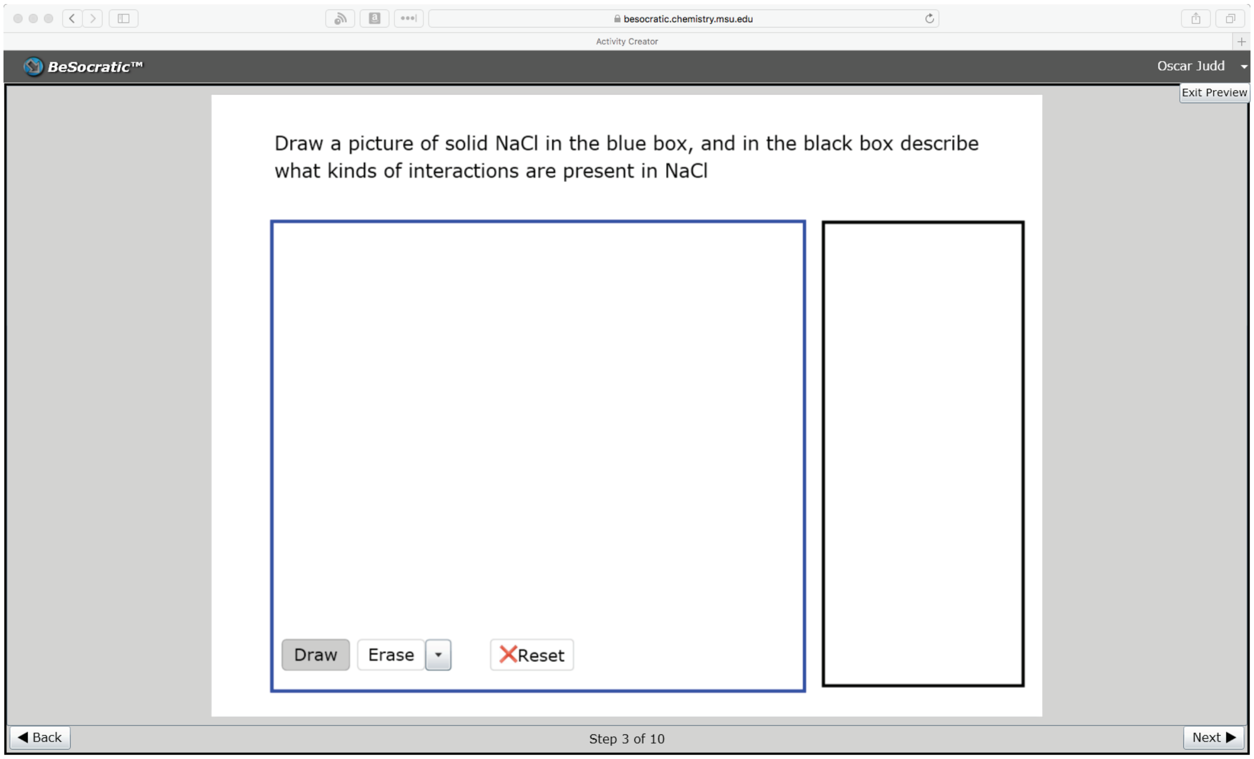


Figure A.2 — Representation prompt for undissolved sodium chloride

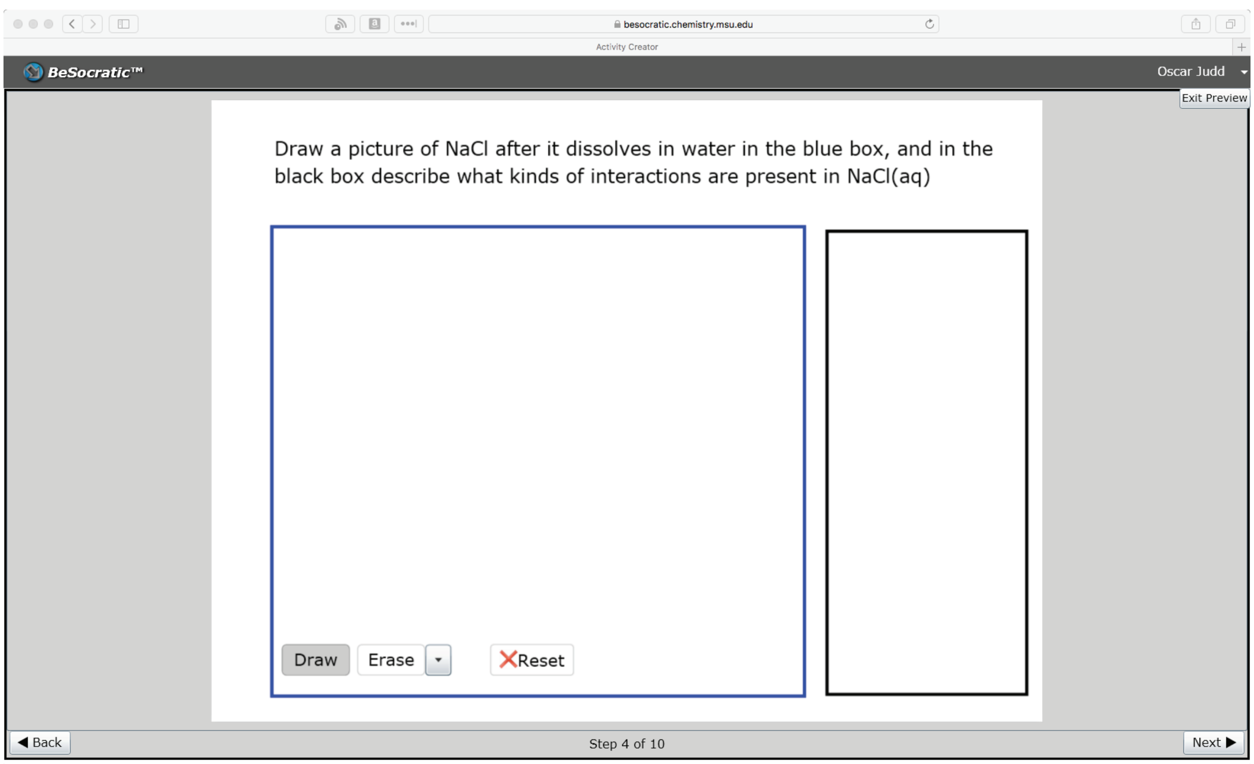


Figure A.3 — Representation prompt for aqueous sodium chloride

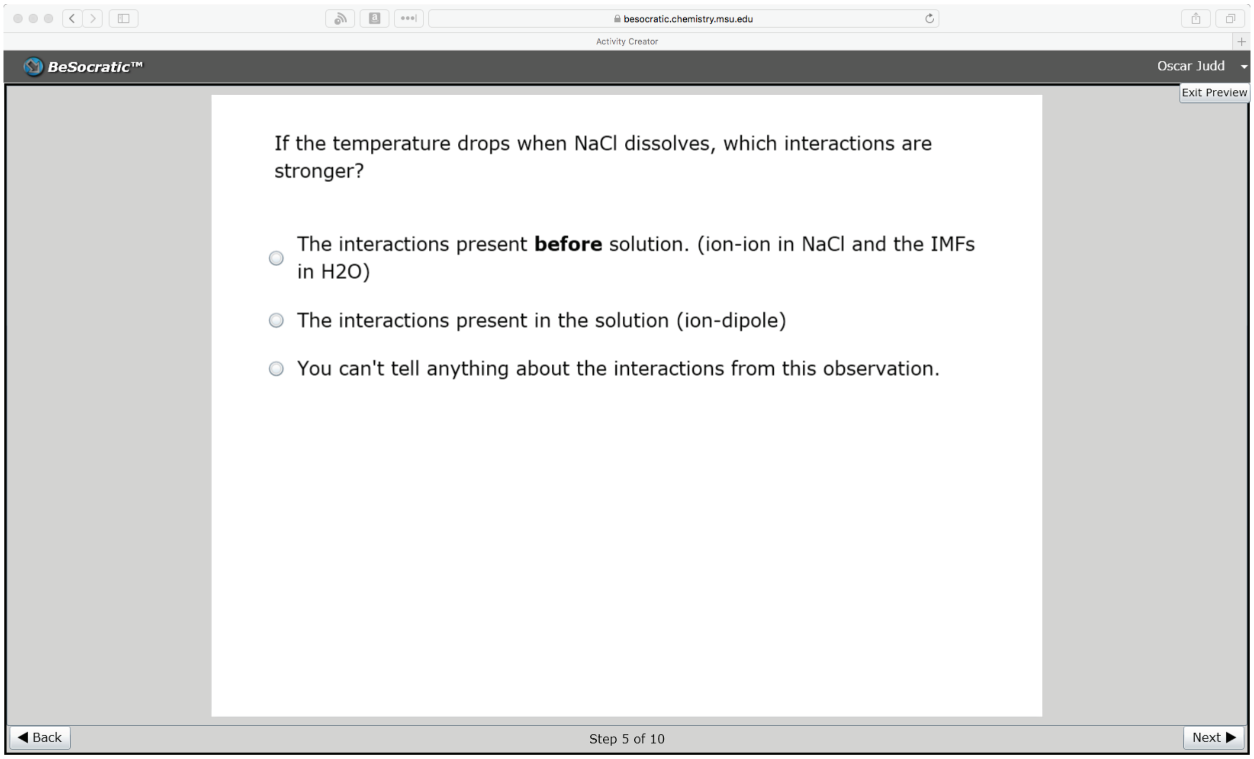


Figure A.4 — Comparison of strengths of interactions question

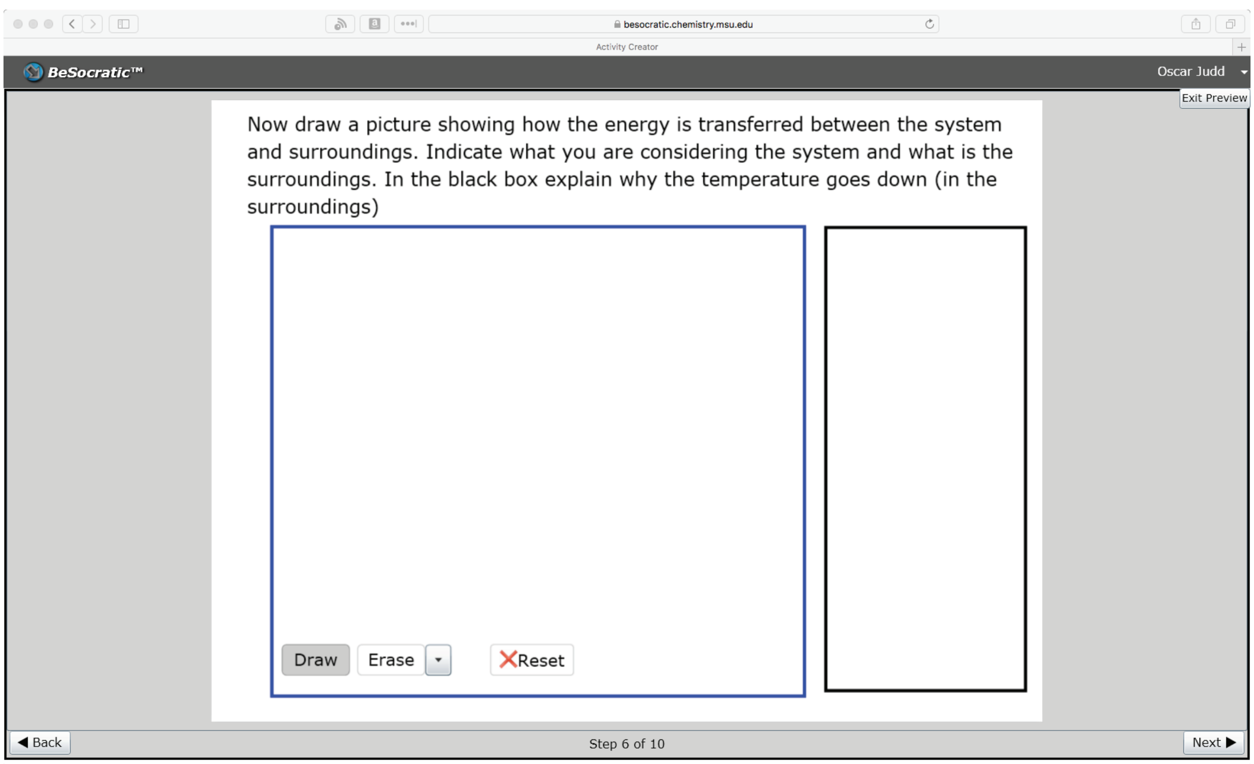


Figure A.5 — Representation prompt for mechanism of energy transfer

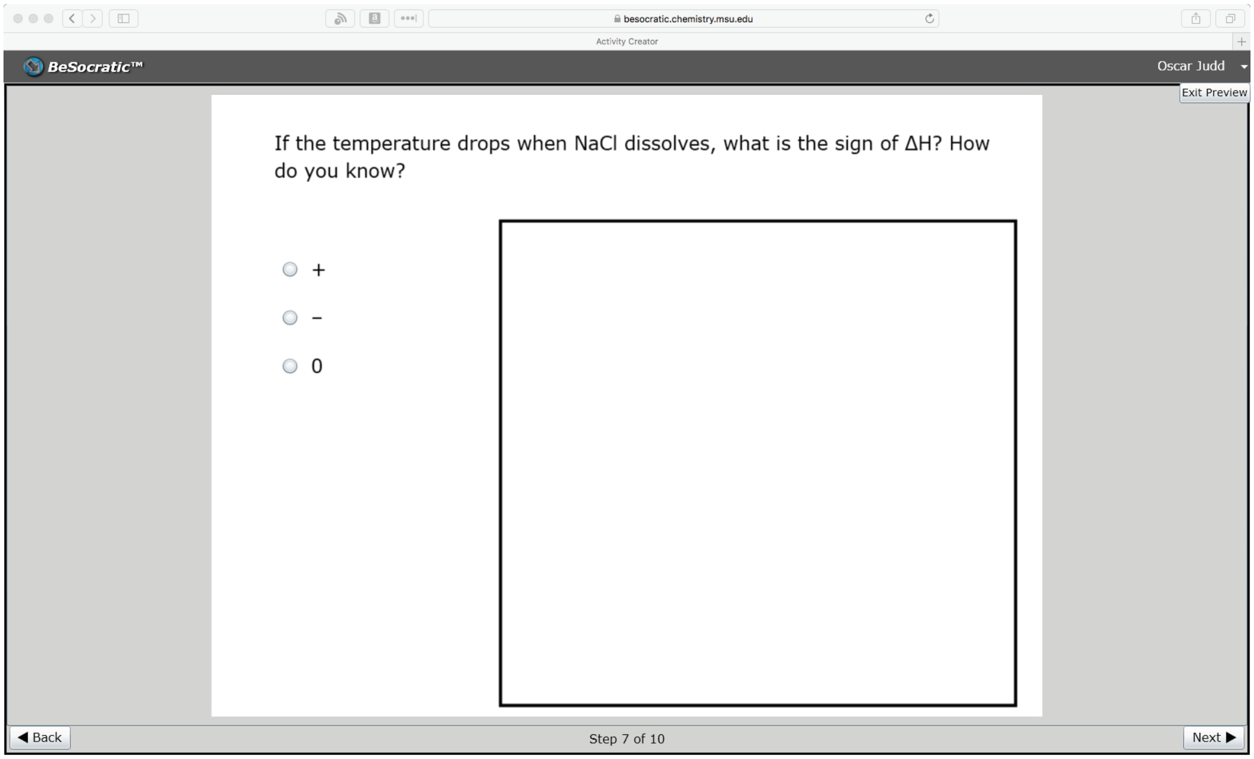


Figure A.6 — Predict and explain enthalpy change prompt

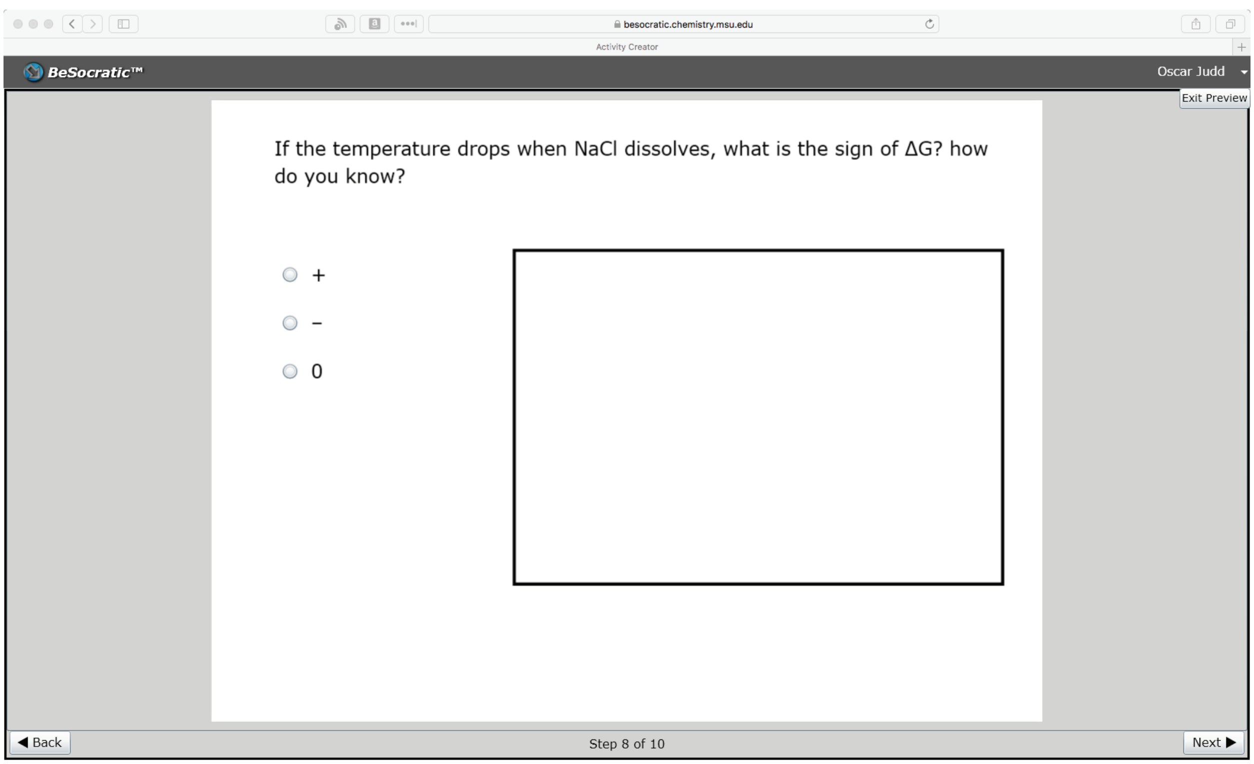


Figure A.7 — Predict and explain Gibbs free energy change prompt

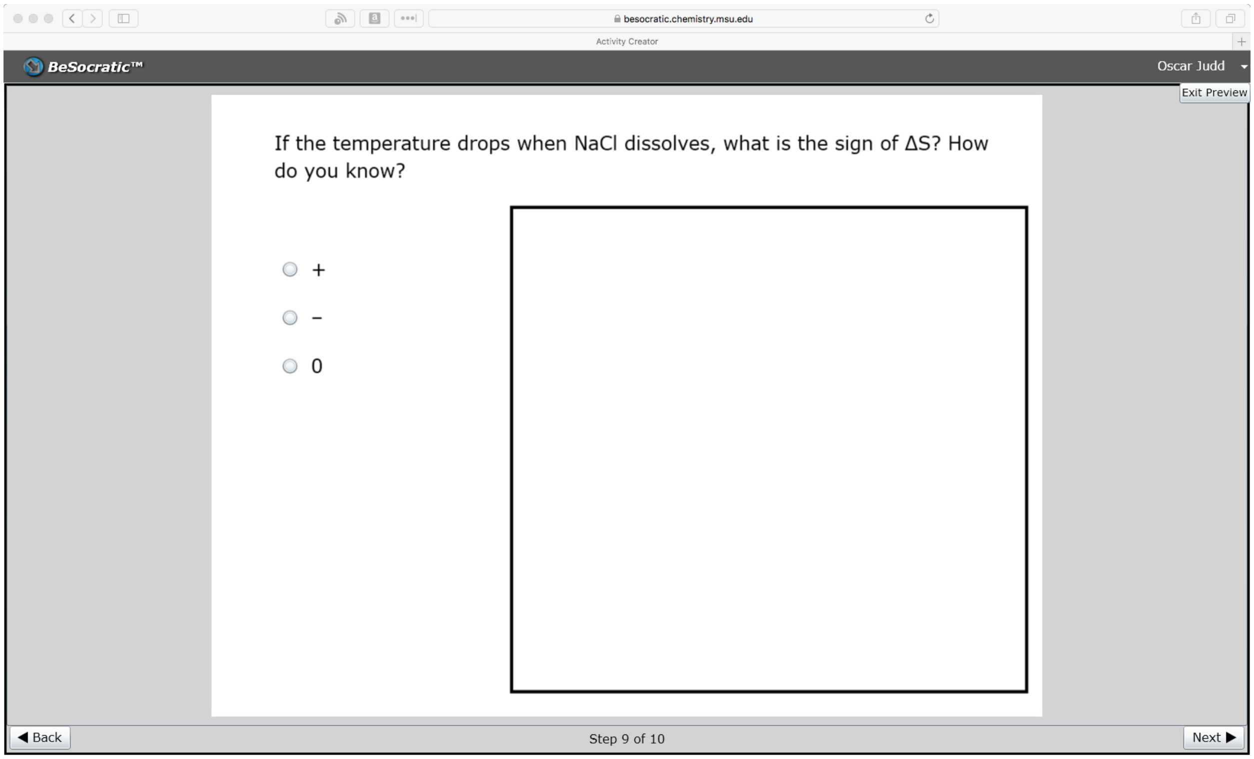


Figure A.8 — Predict and explain entropy change prompt

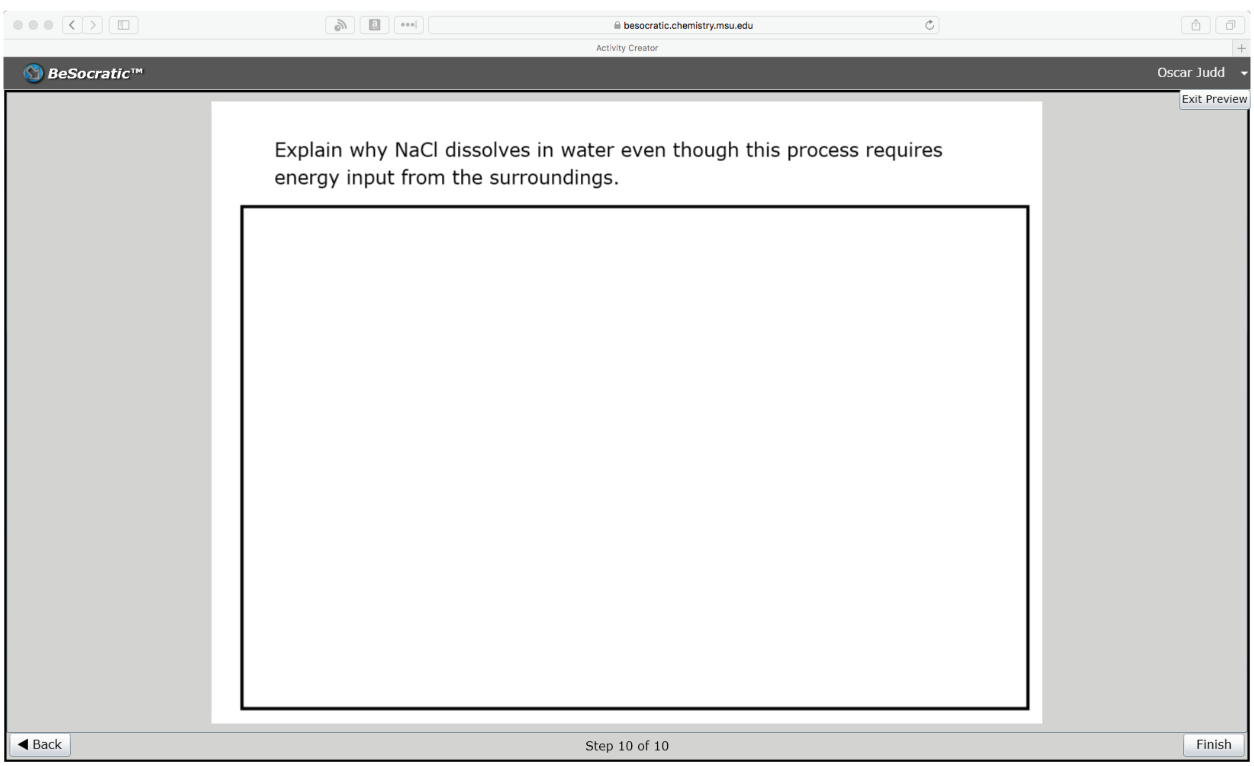


Figure A.9 — Explain entropic and enthalpic contributions to solubility of sodium chloride prompt

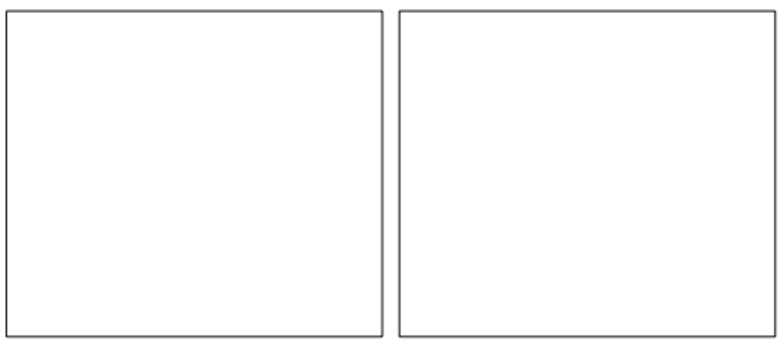
APPENDIX B — INTERVIEW PROTOCOL: INVESTIGATING STUDENT UNDERSTANDING OF CONNECTIONS BETWEEN MACROSCOPIC ENERGY AND CHANGES AT THE ATOMIC-MOLECULAR LEVEL

Part 1: A

Imagine you have a mixture of liquid water and water vapor in a beaker at a temperature of 75°C.

You begin heating the water at a constant rate.

Molecular-Level Picture



Before 100°C After 100°C

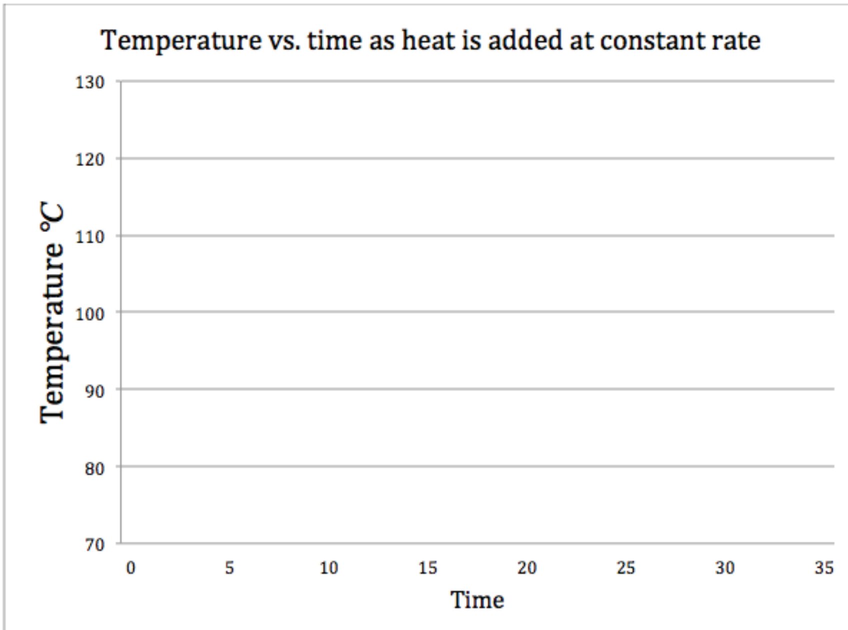
Follow-up questions and prompts for further explanation:

- Describe what you think will happen?
  - What's the system? What happens to the system? Surroundings?
  - At the molecular level?
- Sketch a molecular-level representation of the change as temperature increases above 100°C (show species present before and after change);
  - What forces/interactions between particles are present before heating? How are the molecules interacting? Spacing of particles?
  - What are interactions between particles like after?

Figure B.1 — Student prompt and interviewer protocol for item 1A: Representing water as a liquid and a gas

Part 1: B
Imagine you have a mixture of liquid water and water vapor in a beaker at a temperature of 75°C.

You begin heating the water at a constant rate.

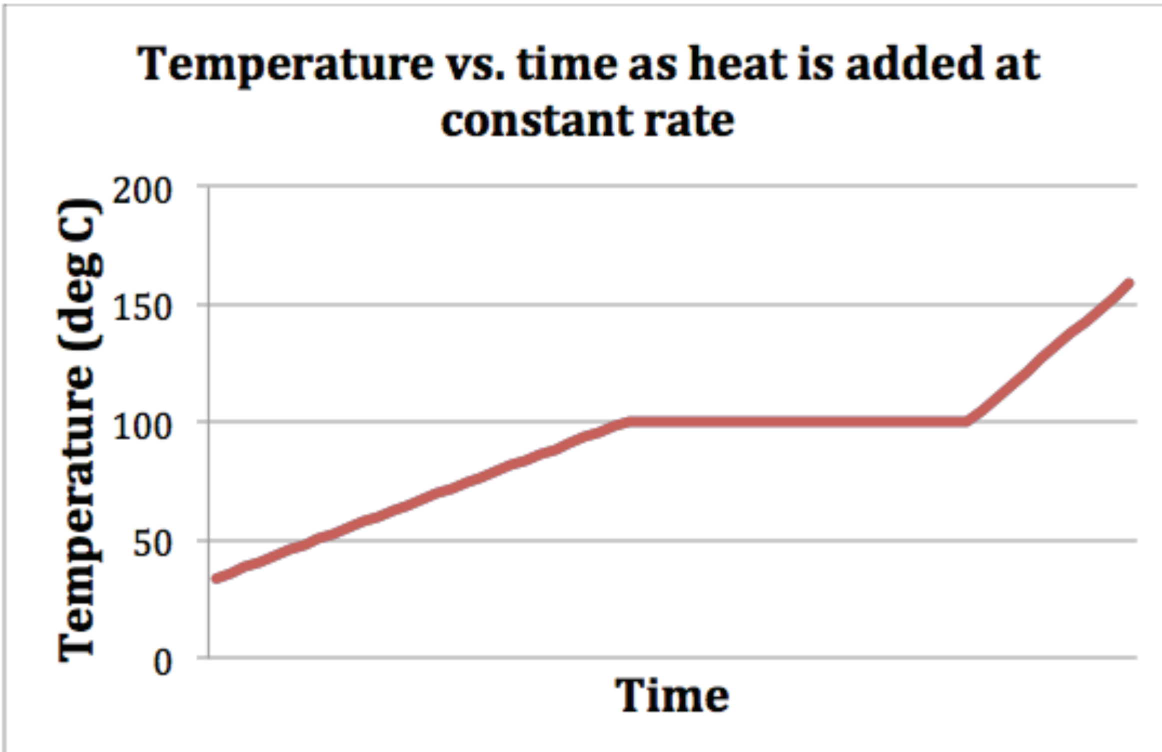


Follow-up questions and prompts for further explanation:

- Sketch a graph to show how the temperature of the sample would change as heat is added to the sample of water.
    - The axes have been labeled for you
    - Explain what's going on at each segment of the curve.
    - Sketch what you think is happening at the molecular level for each part of the curve
    - On the plateau, the temperature is no longer changing, even though heat is still added. Explain this observation.

Figure B.2 — Student prompt and interviewer protocol for item 1B: Generating a heating curve for a sample of water

Part 1: C (Follow-up)



Follow-up if they have difficulty drawing:

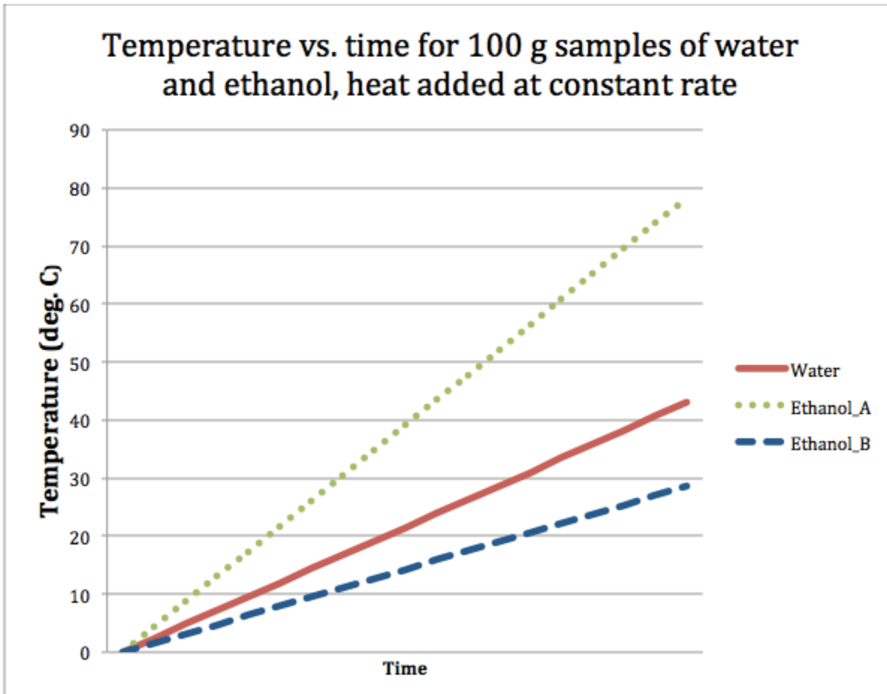
- Here's a heating curve that was drawn by another student.
    - Describe what's going on in the diagram?
    - Explain what's going on at each segment of the curve.
        - Sketch what you think is happening at the molecular level for each part of the curve
    - How does it compare to the one you drew? Could this be correct? Why or why not?
    - On the plateau, the temperature is no longer changing, even though heat continues to be added. Explain this observation.

Figure B.3 — Student prompt and interviewer protocol for item 1C: Follow up to item 1B if students have difficulty generating a heating curve

Part 1: D
The solid line below represents temperature change in a 100 g sample water when heat is added at a constant rate, beginning from 0 °C.

One of the dotted lines represents temperature change in a 100 g sample of ethanol (CH_3CH_2OH)

Which line do you think it is?



Follow-up questions and prompts for further explanation:

- If you look at the graph. At the ending point, the same amount of heat has been added to each substance, but the temperature is not the same. Explain why you think this is?
- If they mention heat capacity of water, why are the heat capacities of ethanol and water different? (explain at the molecular level); why are there more IMF in water?

Figure B.4 — Student prompt and interviewer protocol for item 1D: Prediction of a heating curve

Part 2A

In a beaker, you mix 500 mL of water and 50 g of KCl, a white solid.

You observe that the white solid dissolves and that the temperature increases.

Explain these observations.

Follow-up questions and prompts for further explanation:

- Explain why you think the temperature increases upon mixing.
- What does the term exothermic reaction mean to you? Why would heat be released?
- What happens at the molecular level?
- Draw a molecular level picture: before and after dissolving the KCl?
- If system/surroundings mentioned – describe what you mean by system and surroundings here?
- If "stored" energy – why do you say energy is stored.
    - How does the observed temperature change relate to changes in kinetic and potential energy as the species interact?

Figure B.5 — Student prompt and interviewer protocol for item 2A: Explaining a temperature change occurring with solution formation

Part 3A
The enthalpy change for another reaction is $\Delta H_{rxn} = -706\ kJ/mol$. The reaction is shown below.

$$CH_4\ (g) + O_2\ (g) \rightarrow CO_2\ (g) + H_2O\ (g)$$

Draw a molecular-level picture to show what processes are responsible for the energy change that accompanies this reaction.

Before | After

Follow-up questions and prompts for further explanation:

- What does the term $\Delta H_{rxn} = -706\frac{kJ}{mol}$ mean to you?
- Draw a molecular-level picture to show what processes are responsible for the energy change that accompanies this reaction.
- How would you explain your answer using your understanding of the forces and energy changes that are involved in bond formation.
- If "stored" energy – why do you say energy is stored.
    - How does the observed temperature change relate to changes in kinetic and potential energy as the species interact?
- IF they don't bring up PE, you mentioned interactions: Sometimes we'll talk about PE as stored via interactions between atoms and molecules
    - What do you think that means?
    - How does the observed temperature change relate to changes in kinetic and potential energy as the species interact?
    - Earlier in the semester we talked about PE changes as atoms and molecules interact. Now we're talking about energy changes as chemical reactions occur. Can you tell me about your understanding of the relationship between those ideas?

Figure B.6 — Student prompt and interviewer protocol for item 3A: Representing and explaining the enthalpy change of a chemical reaction with molecular-level representations

Part 3B
Sketch an energy diagram showing the relative energy levels of products and reactants.

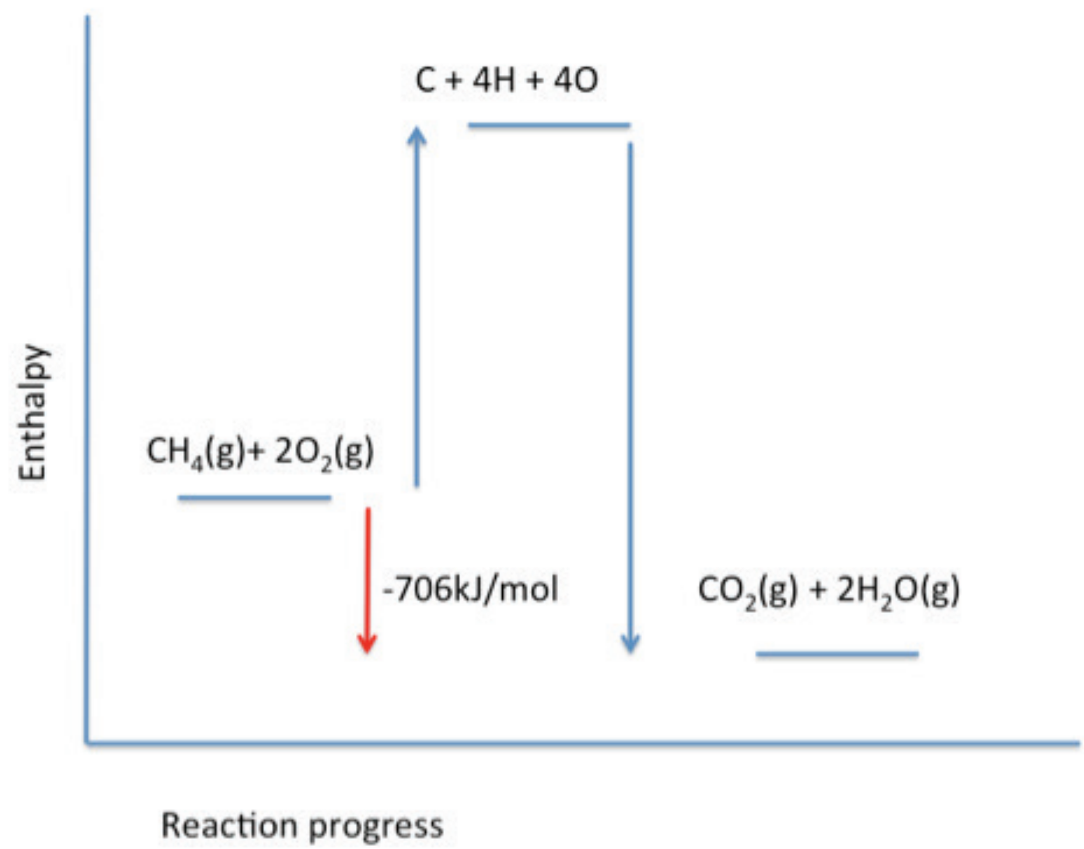
$$CH_4\ (g) + 2O_2\ (g) \rightarrow CO_2\ (g) + 2H_2O\ (g) \quad \Delta H_{rxn} = -706\ kJ/mol$$

Follow-up questions and prompts for further explanation:

- Draw an energy diagram showing the relative energy of the reactants and products.
- Discuss interpretation of the drawing

Figure B.7 — Student prompt and interviewer protocol for item 3B: Representing and explaining the enthalpy change of a chemical reaction with an energy level diagram

Part 3C (Follow-up)



Follow-up questions and prompts for further explanation:

- Here's a diagram that was drawn by another student.
  - Can you tell me what you think is going on in this diagram?
  - How does it compare to the one you drew?

Figure B.8 — Student prompt and interviewer protocol for item 3C: Follow up to item 3B if students have difficulty generating energy level diagram

APPENDIX C — FINAL VERSION OF REVISED FORMATIVE ASSESSMENT ACTIVITY

The final version of the revised formative assessment activity is presented here in full as it would have been viewed and completed by students in the beSocratic environment.

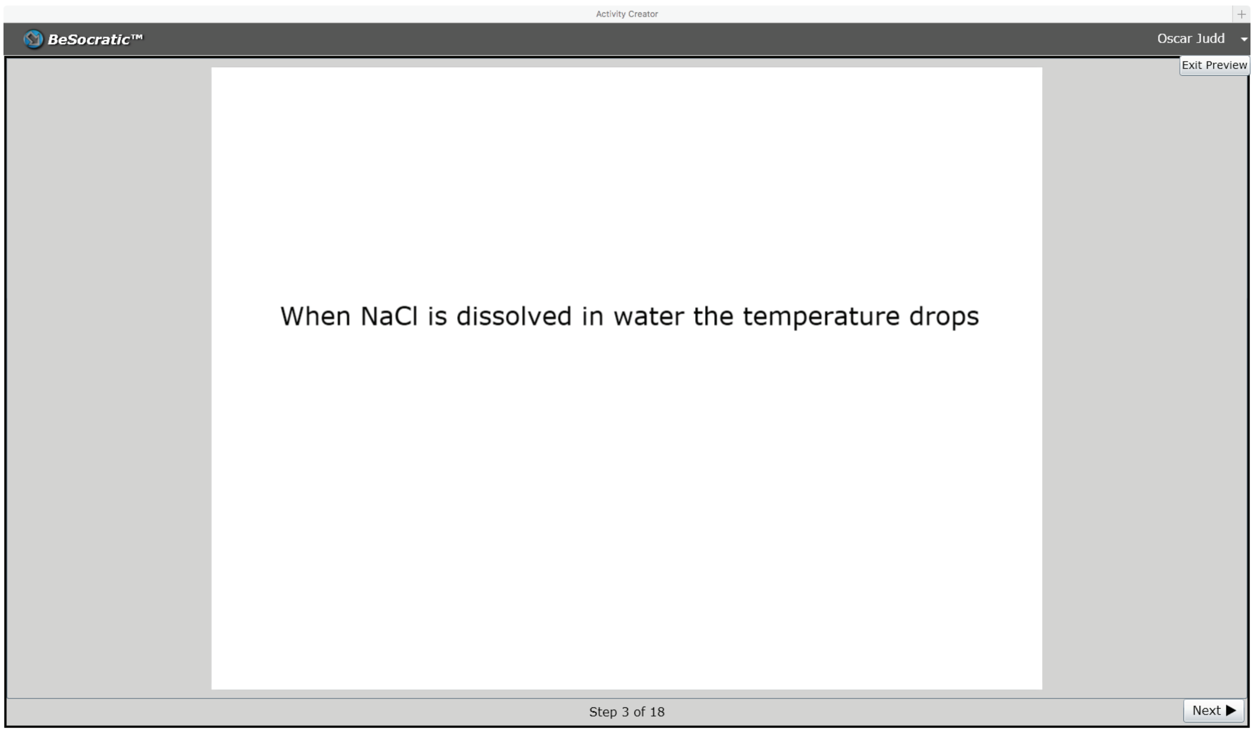


Figure C.1 — Introduction slide

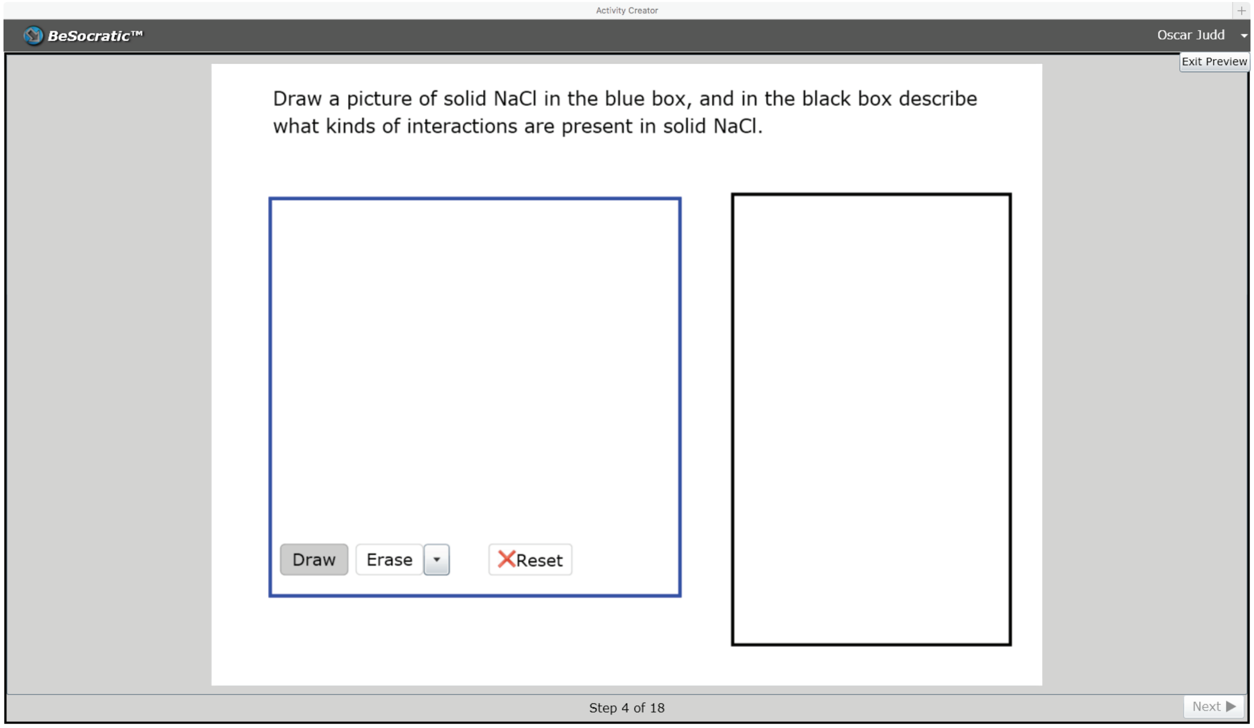


Figure C.2 — Representation prompt for undissolved sodium chloride

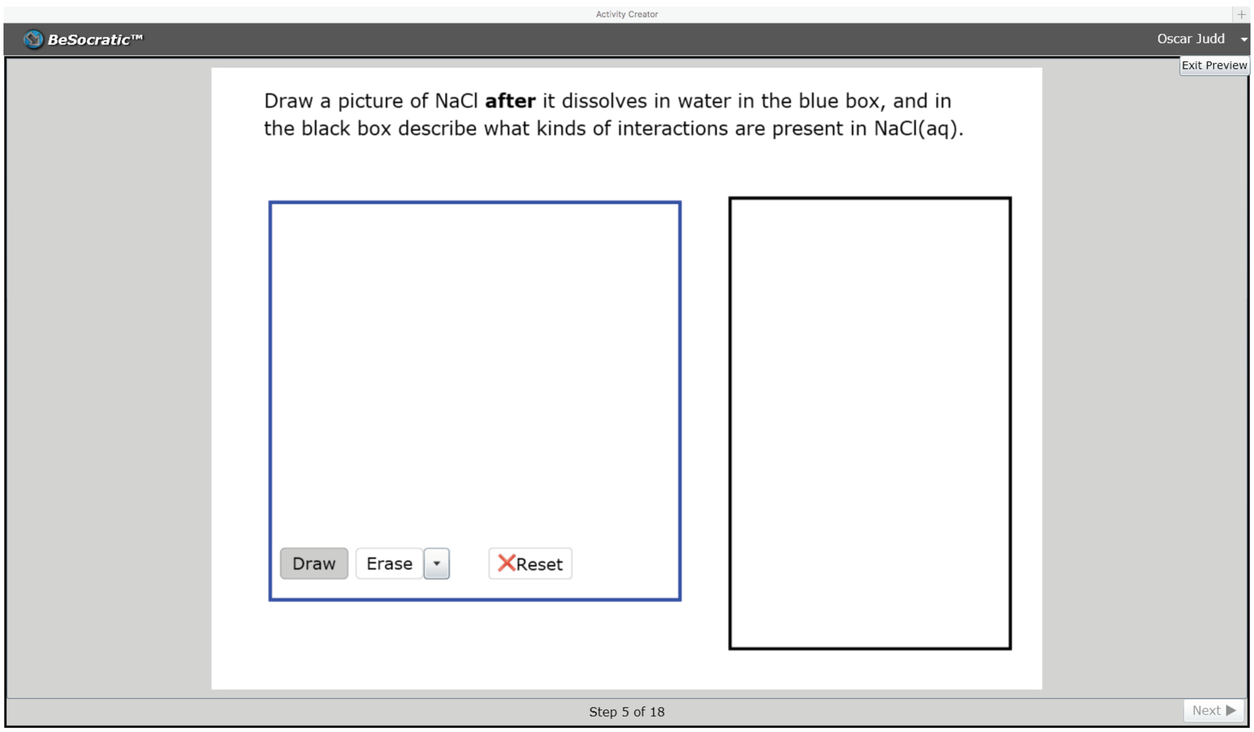


Figure C.3 — Representation prompt for aqueous sodium chloride

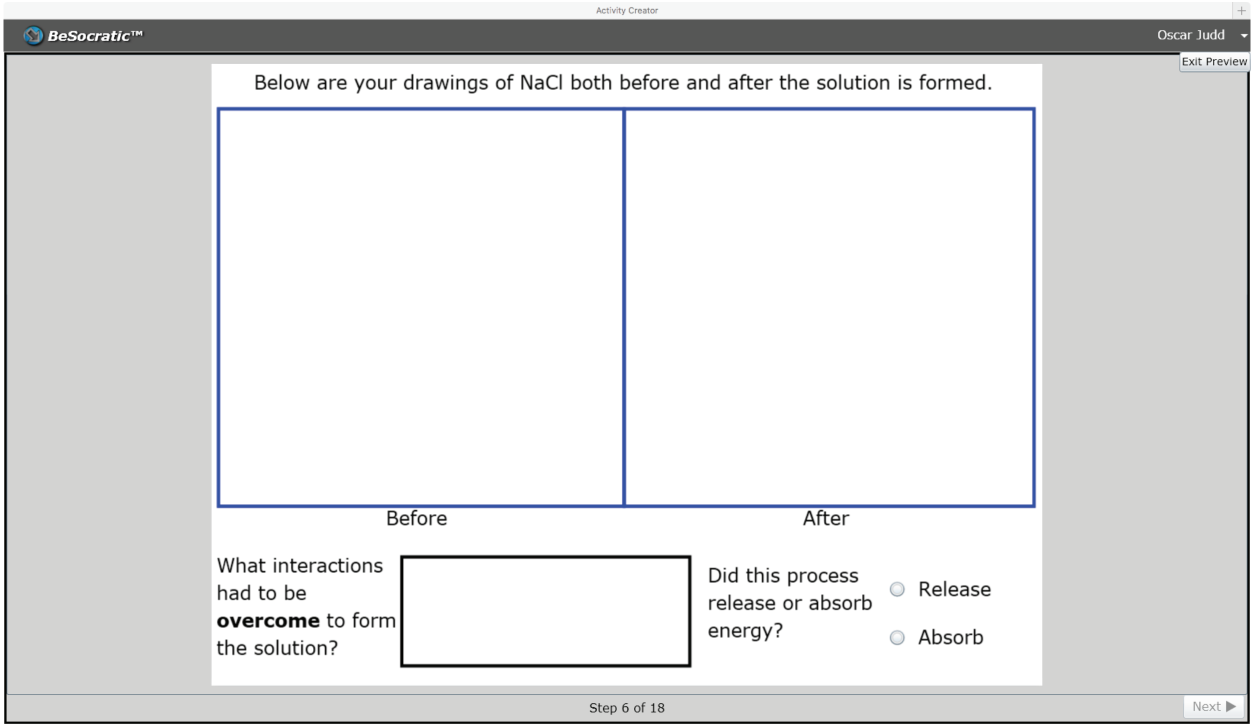


Figure C.4 — Comparison of representations, identification of interactions that have been overcome, and identification of energy flow required to overcome interactions

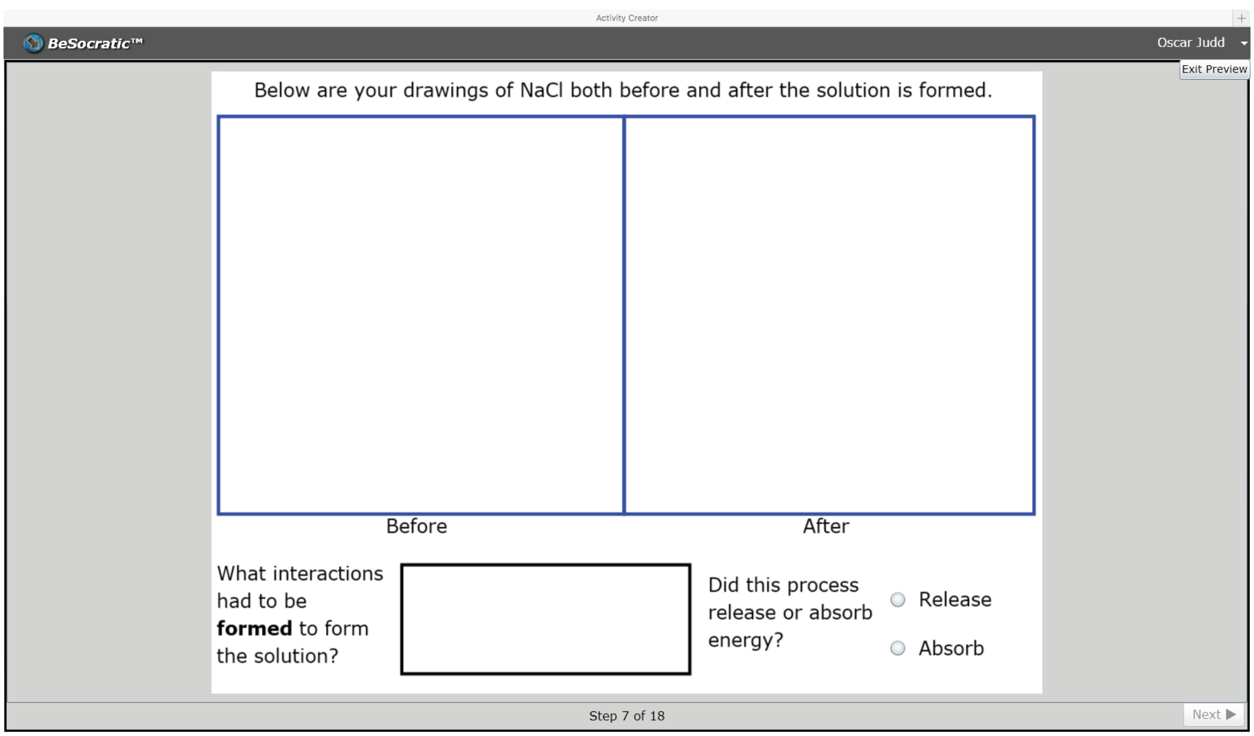


Figure C.5 — Comparison of representations, identification of interactions that have been formed, and identification of energy flow required to form interactions

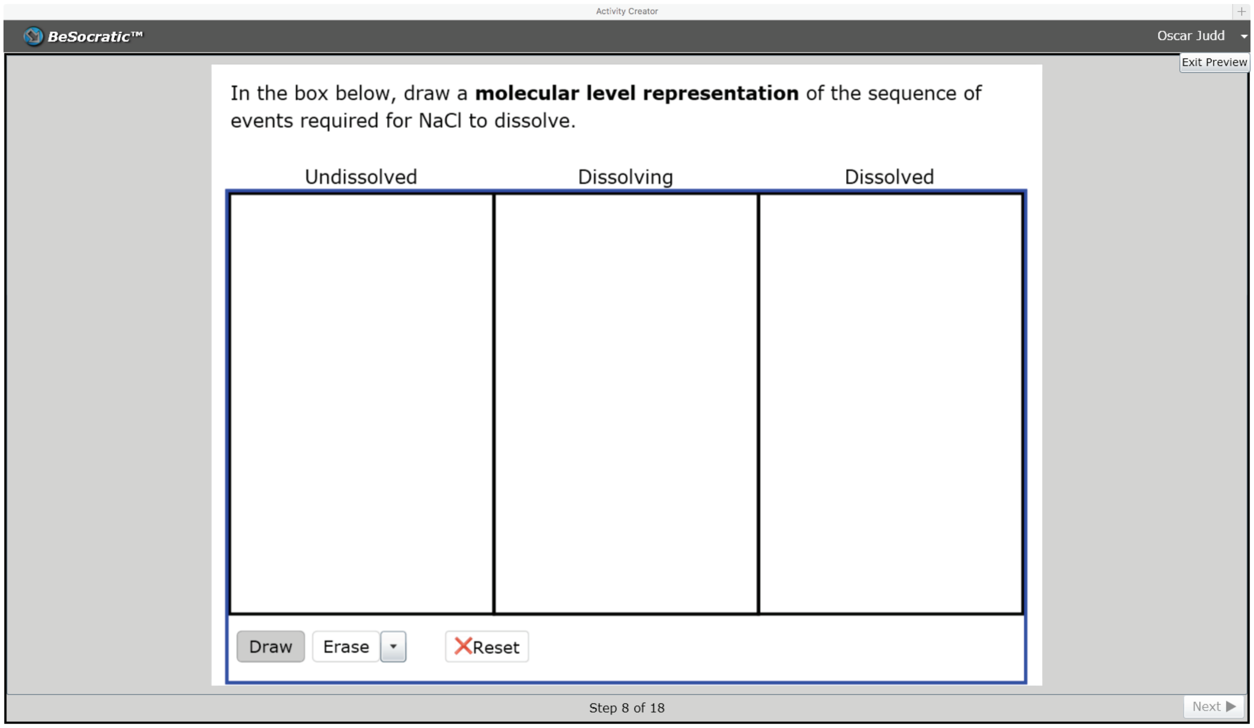


Figure C.6 — Representation of the solvation process prompt

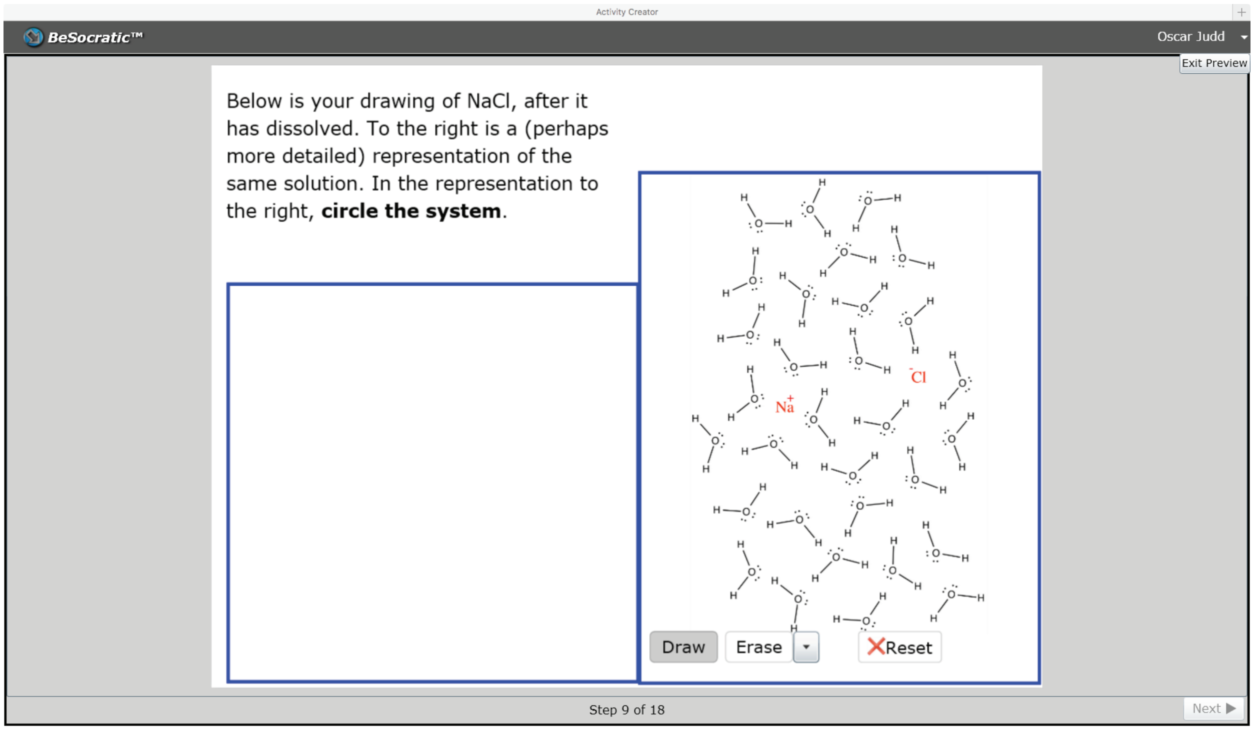


Figure C.7 — Identifying the system

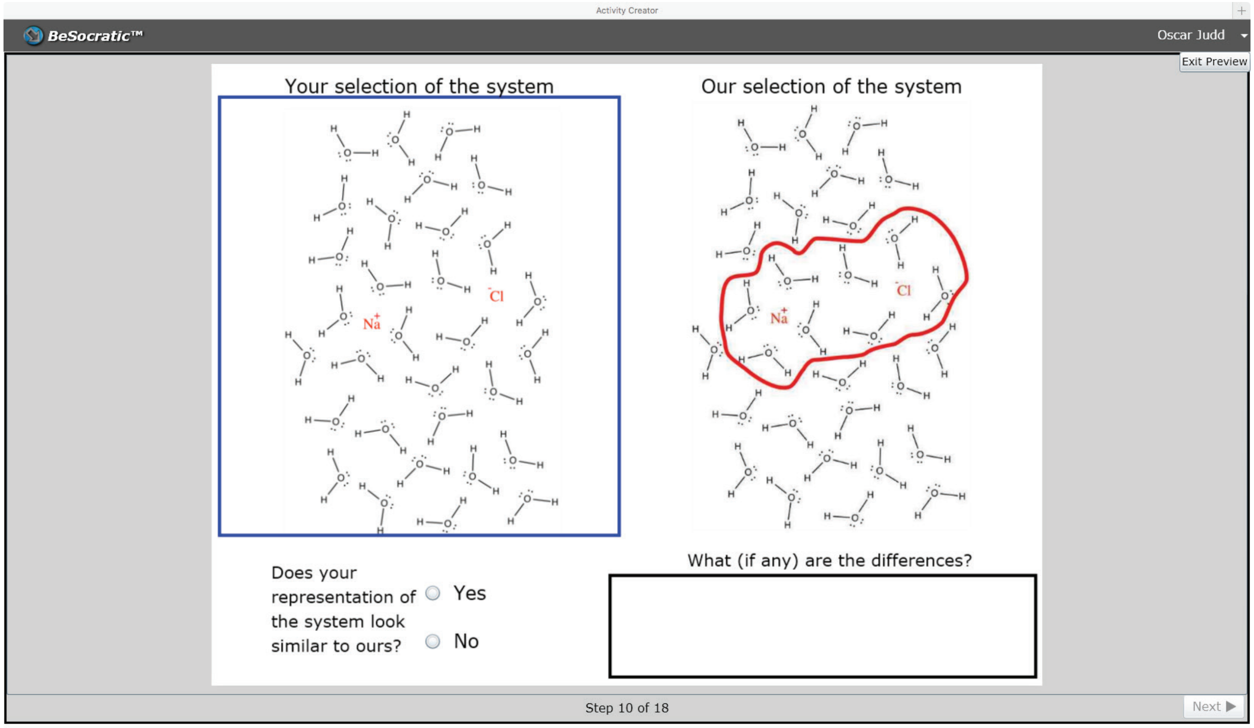


Figure C.8 — Comparison of student's selection of the system to a canonical representation of the system as applicable to the solution formation context

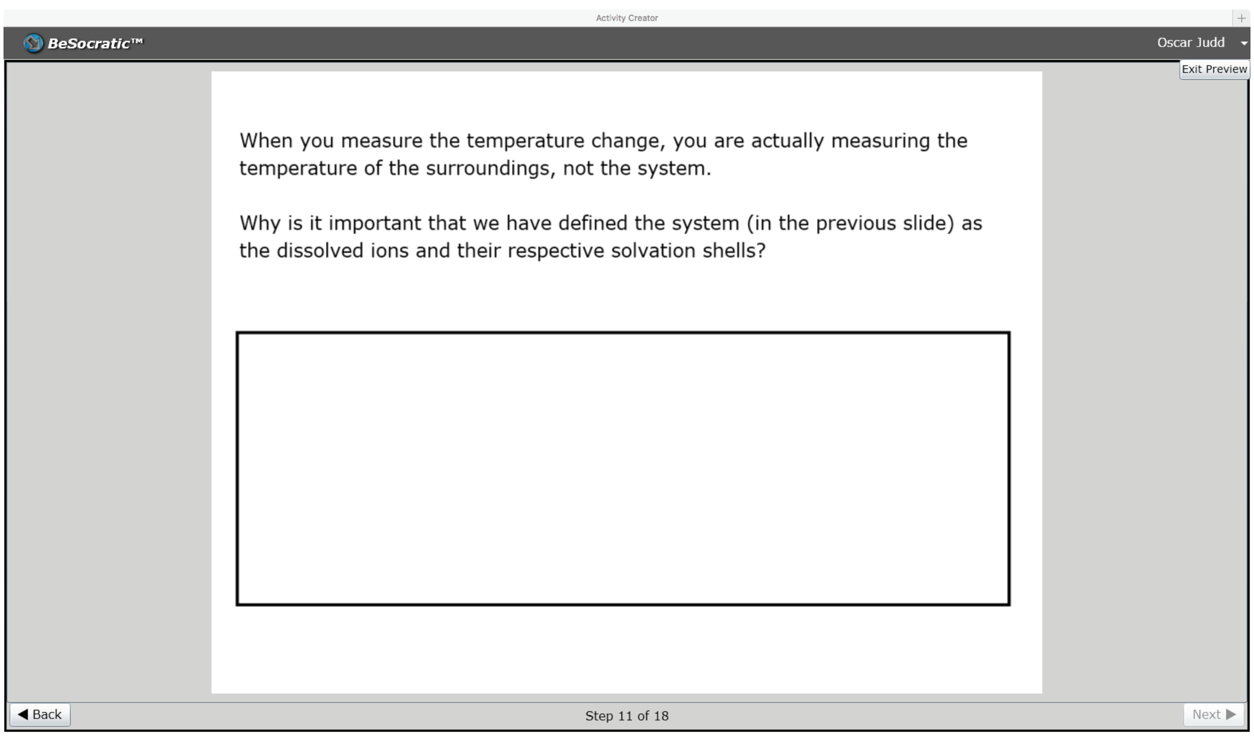


Figure C.9 — Explanation of the importance of defining the system as only the species that are newly interacting after solution formation

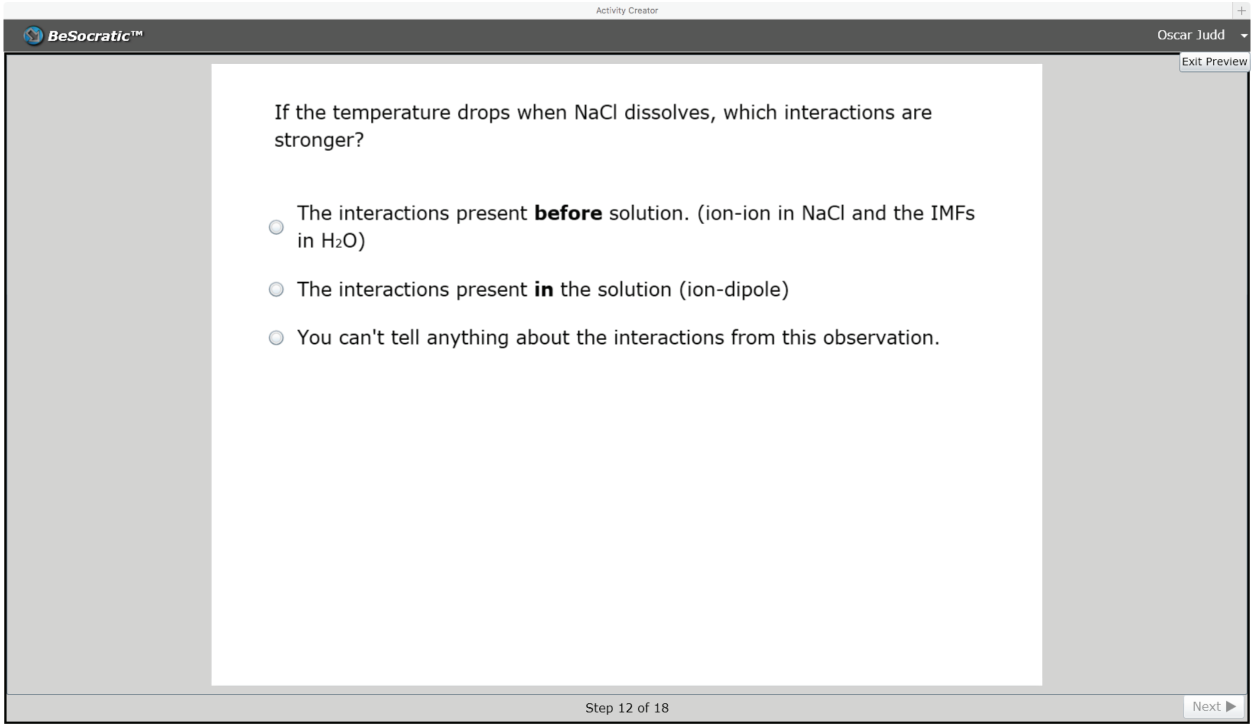


Figure C.10 — Comparison of strengths of interactions question

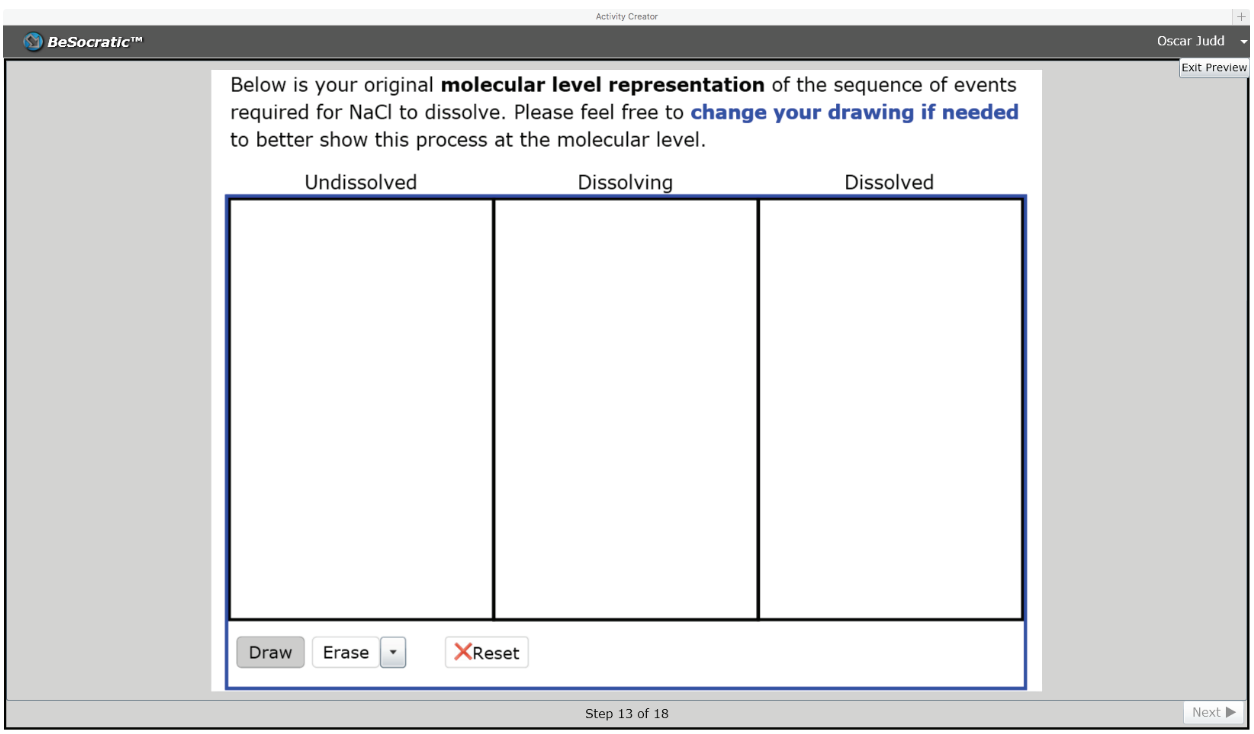


Figure C.11 — Representation of the solvation process prompt revisited, student provided with an opportunity to modify previous representation

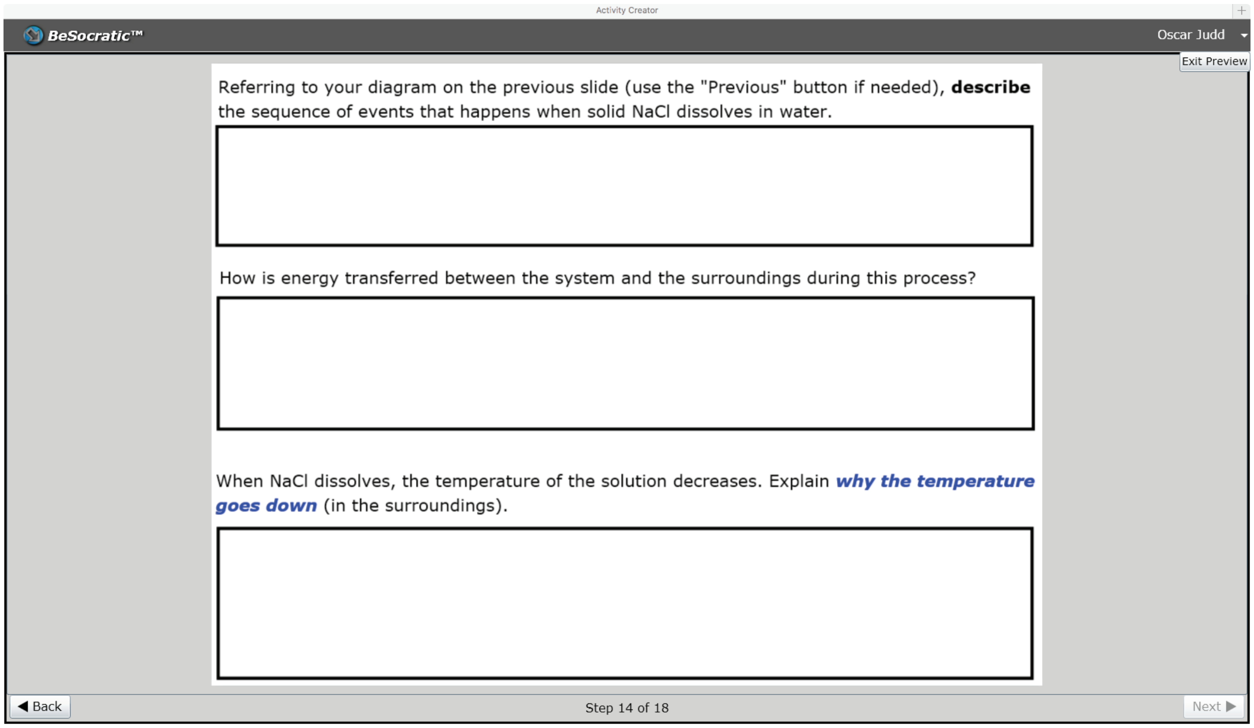


Figure C.12 — Series of questions asking *what* happened when the solution was formed, *how* energy was transferred during solvation, and *why* the temperature decreased

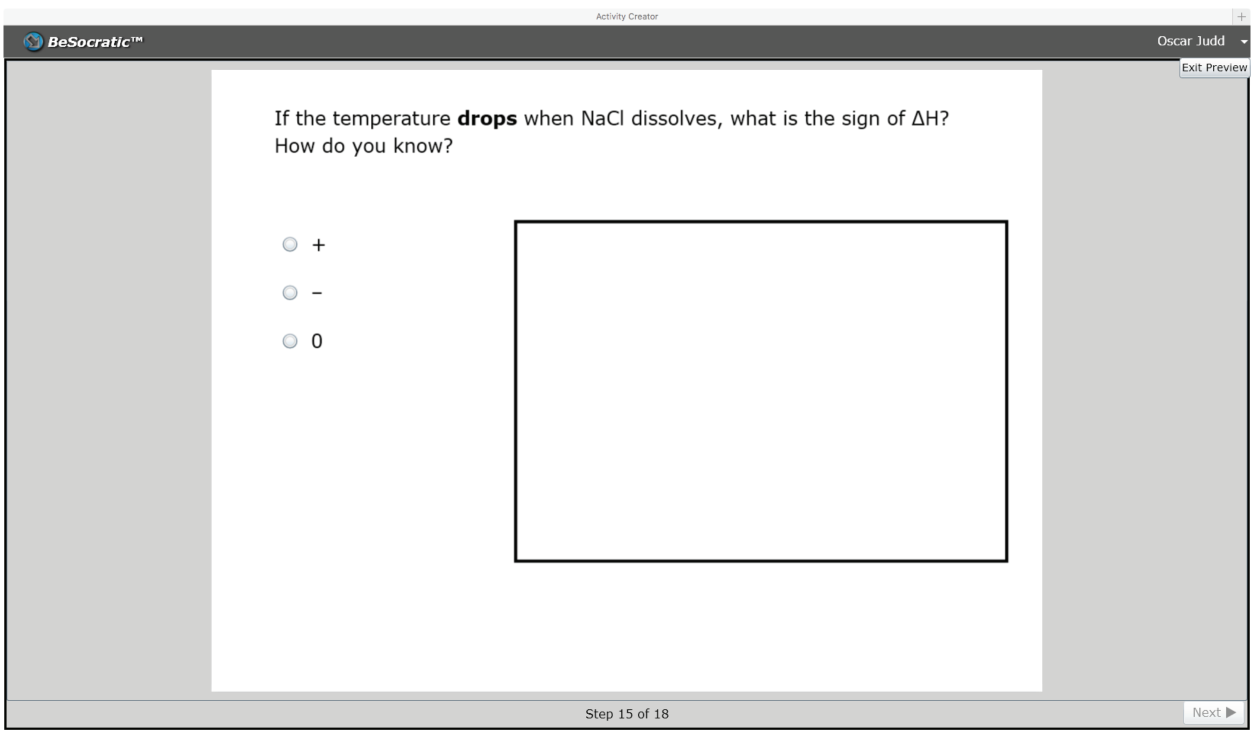


Figure C.13 — Predict and explain enthalpy change prompt

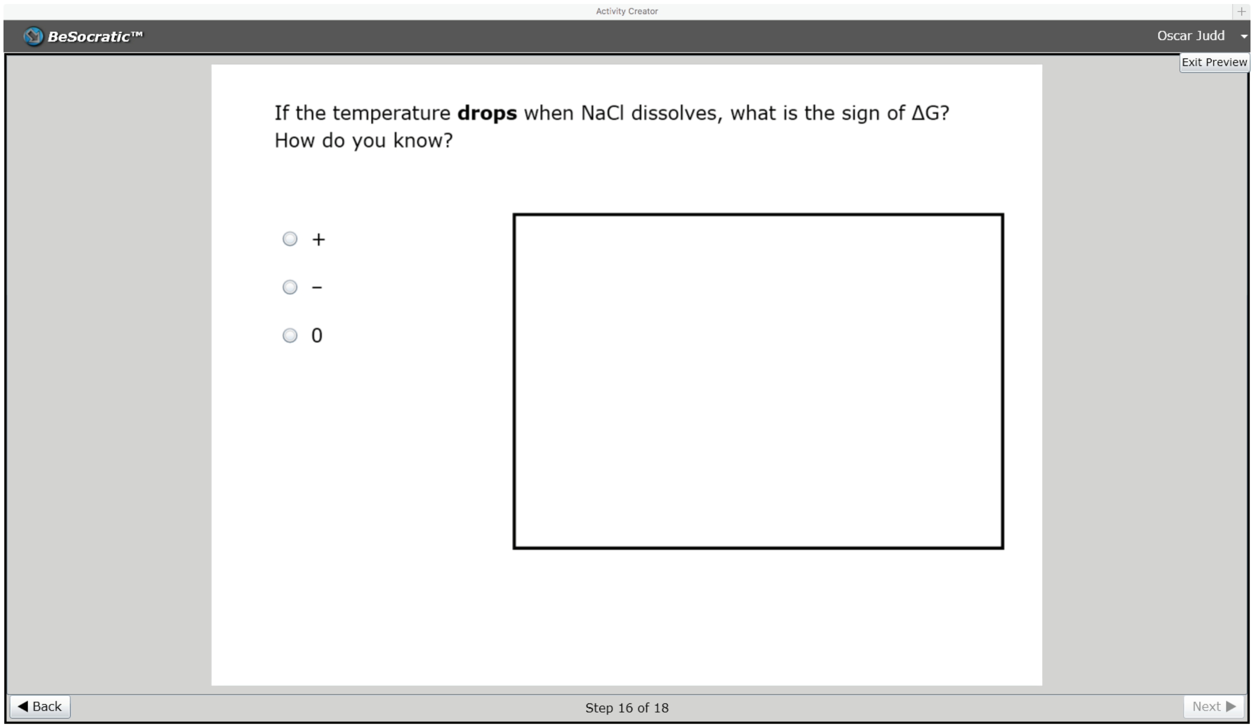


Figure C.14 — Predict and explain Gibbs free energy change prompt

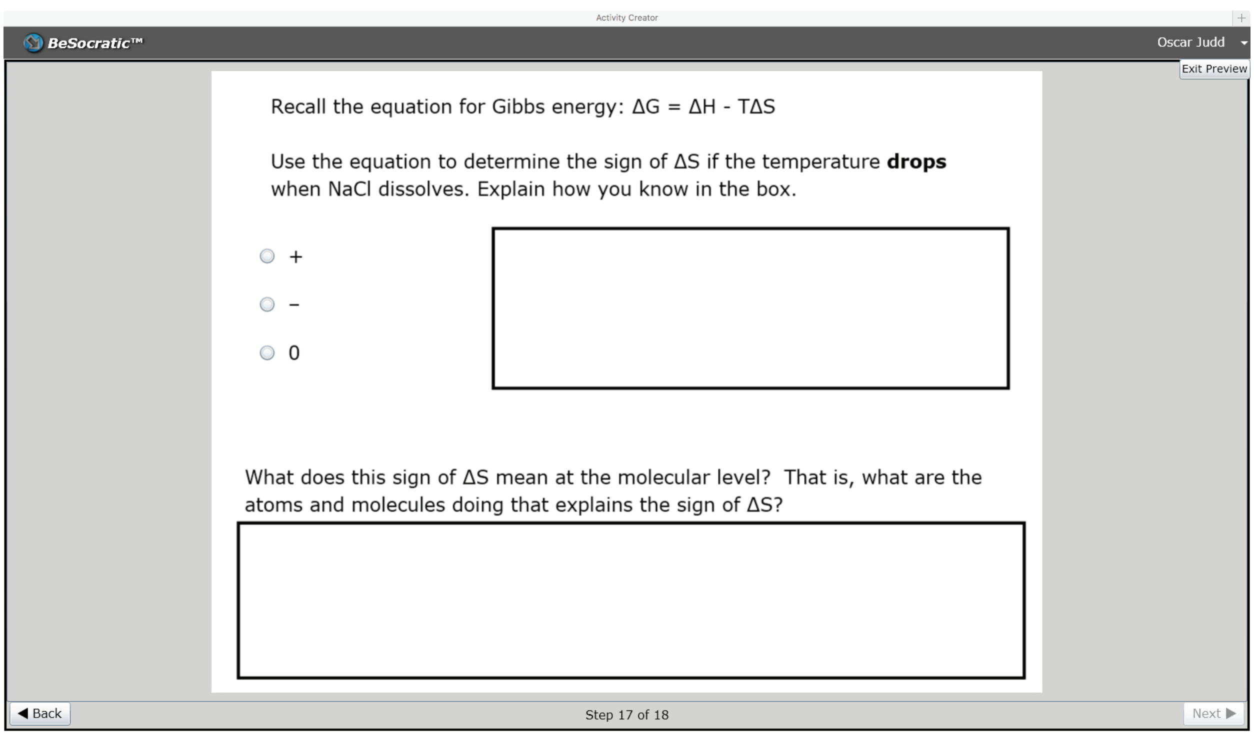


Figure C.15 — Predict entropy change, state how ΔS was determined, and explain conceptually what that change in entropy actually means

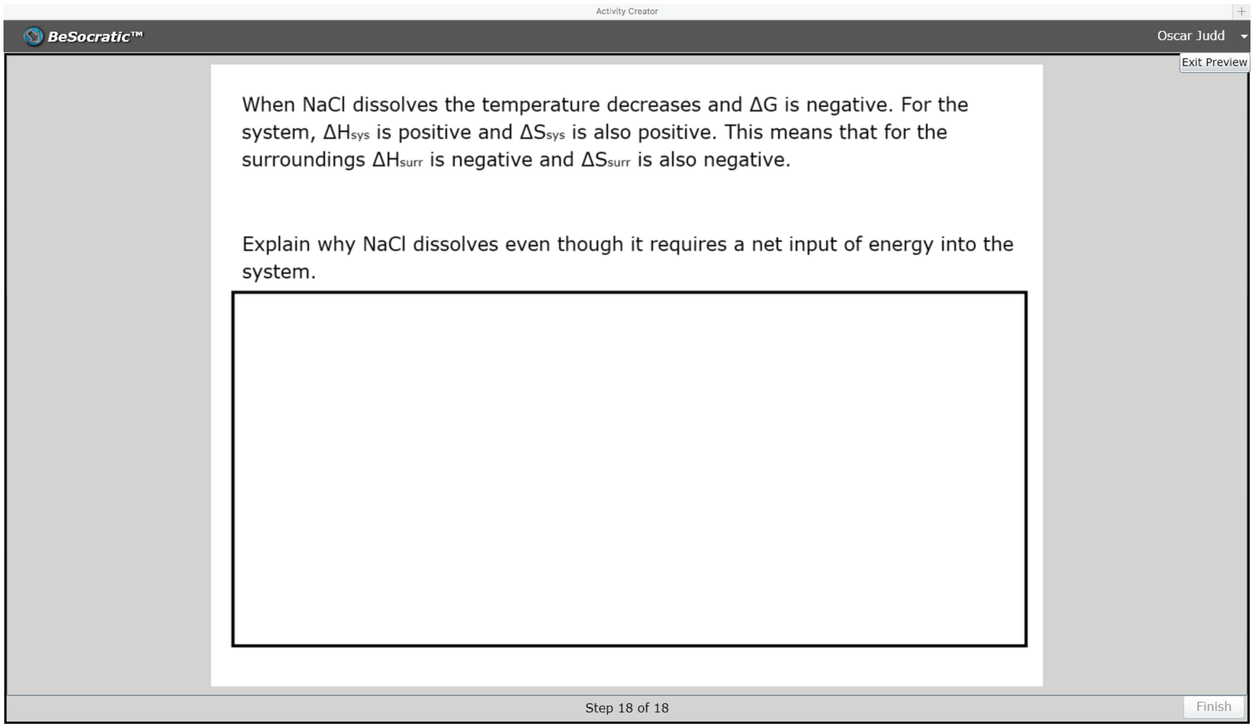
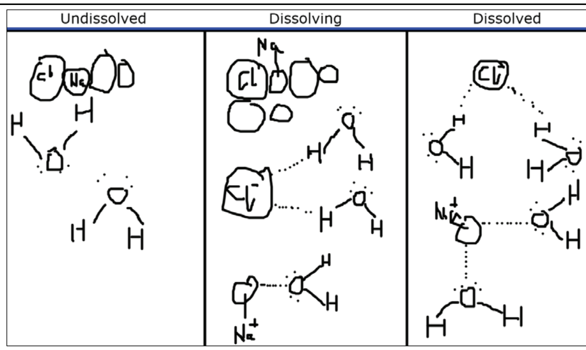
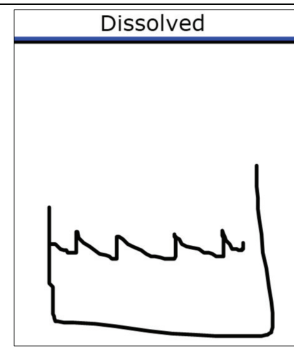


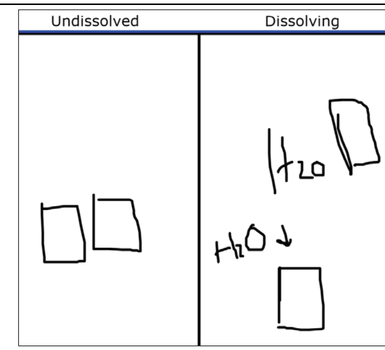
Figure C.16 — Use interaction of entropic and enthalpic contributions to overall ΔG to explain why sodium chloride dissolves even though it requires energy input

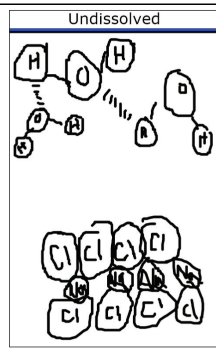
APPENDIX D — INITIAL AND AXIAL CODES GENERATED TO DESCRIBE STUDENT REPRESENTATIONS OF THE SOLUTION PROCESS

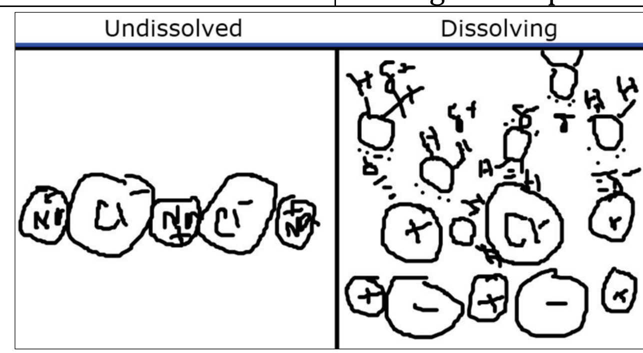
Table D.1 — Codes generated during initial coding of student representations of the solution process

<table>
<tr>
<td>

Atomic-molecular level</td>
<td>

Non atomic-molecular level</td>
<td>

Ambiguous representation of scale</td>
</tr>
<tr>
<td>

First appearance of interactions in “Undissolved”</td>
<td colspan="2">

First appearance of interactions in “Dissolving”</td>
</tr>
</table>

Table D.1 (cont'd)

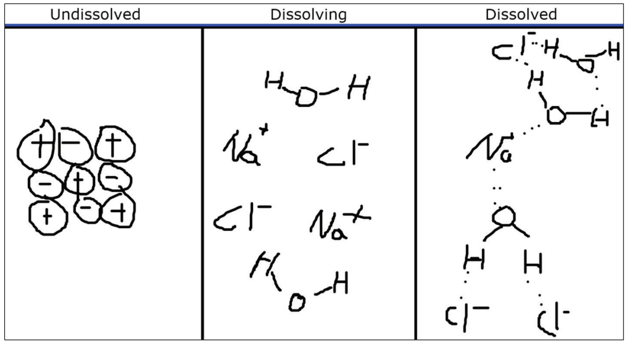
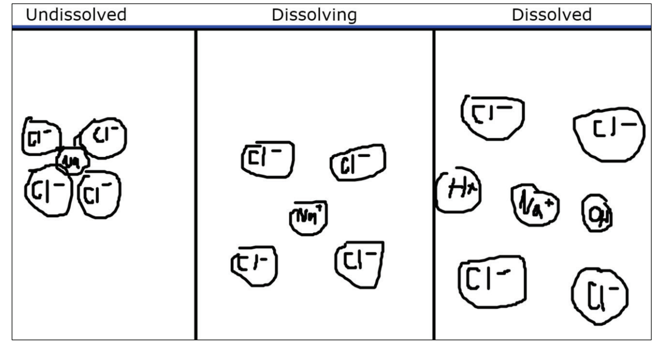
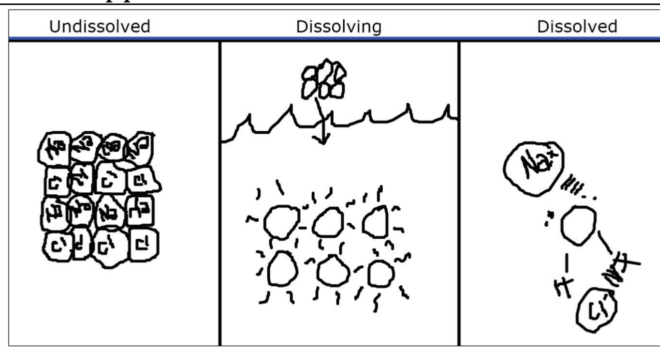
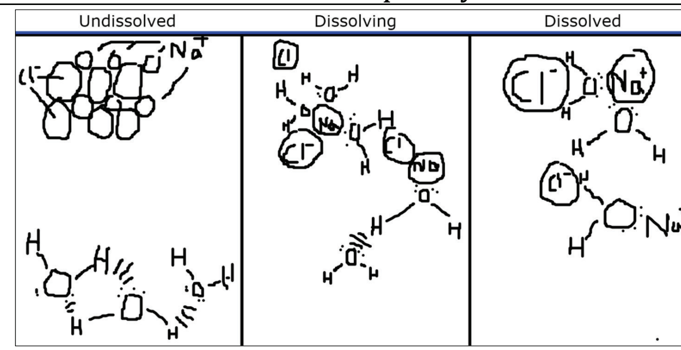
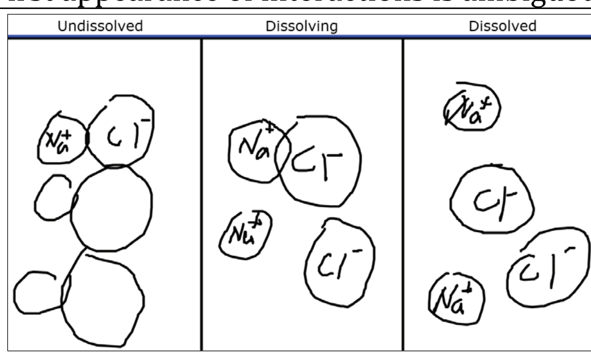
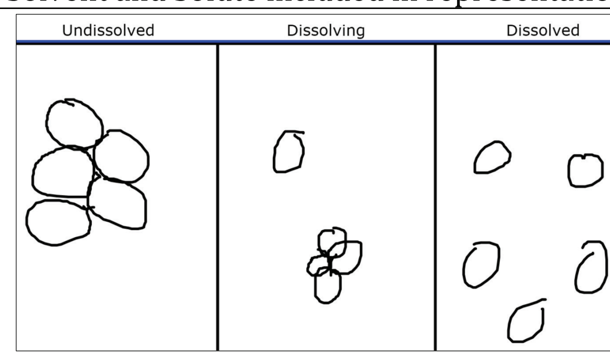
 First appearance of interactions in "Dissolved"	 No interactions explicitly shown
 First appearance of interactions is ambiguous	 Solvent and Solute included in representation
 Solute included in representation	 Components included in representation are ambiguous

Table D.1 (cont'd)

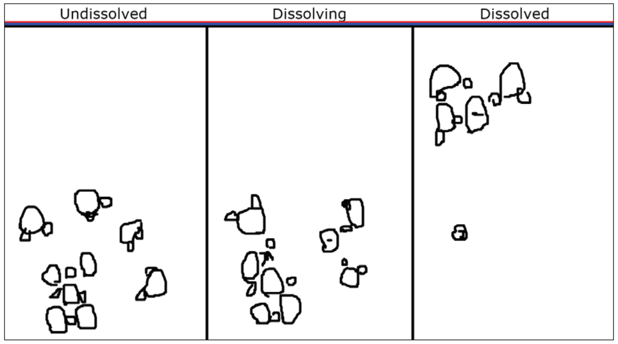
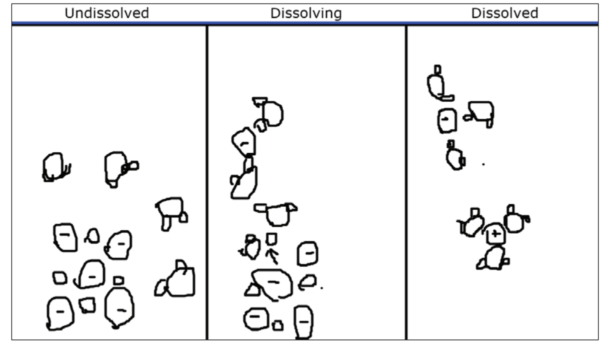
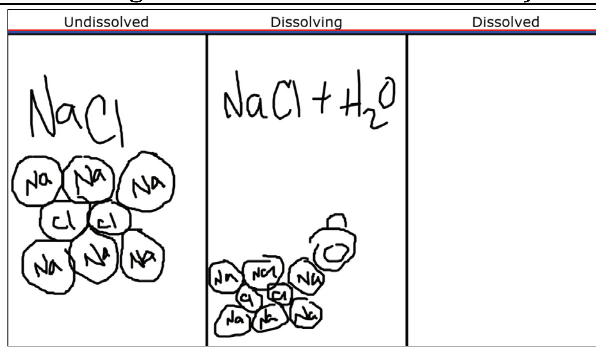
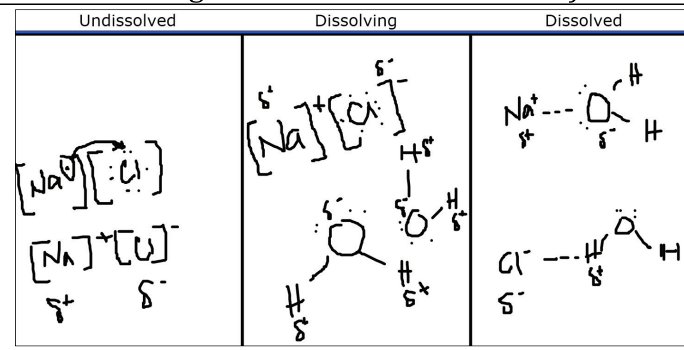
 Drawing tool reset; similar after – *Before*	 Drawing tool reset; similar after – *After*
 Drawing tool reset; different after – *Before*	 Drawing tool reset; different after – *After*

Table D.2 — Axial codes generated and refined to characterize student representation of the solution process

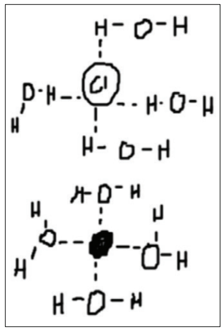
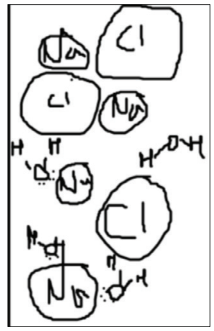
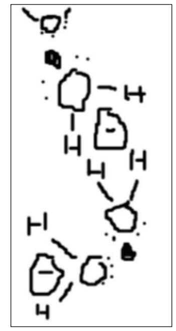
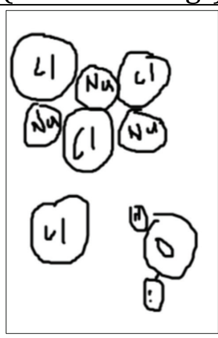
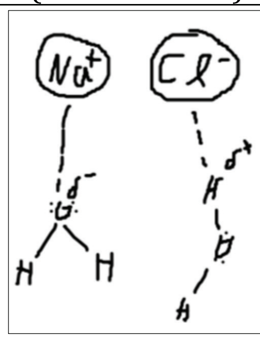
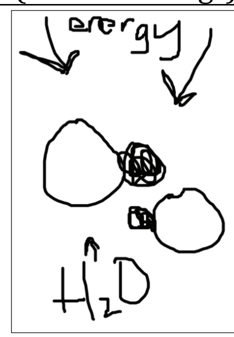
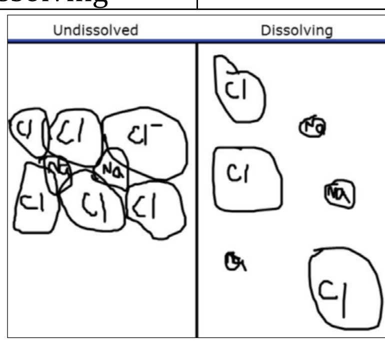
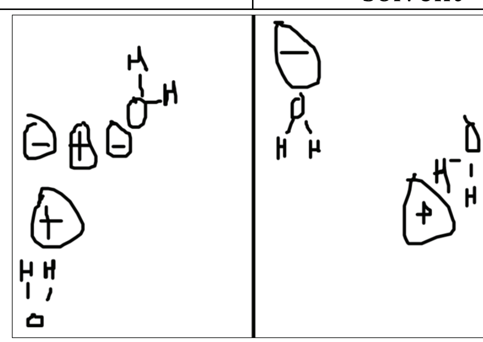
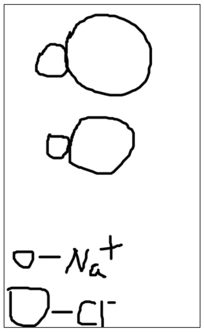
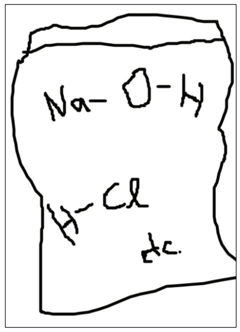
<table>
<tr>
<td>
Explicit interactions (in “Dissolving”)</td>
<td>
Explicit interactions (in “Dissolved”)</td>
<td>
Implicit interactions (in “Dissolving”)</td>
<td>
Implicit interactions (in “Dissolved”)</td>
</tr>
<tr>
<td>
Intact solute included in “Dissolving”</td>
<td>
Solvated ions in “Dissolved”</td>
<td>
Energy added to system</td>
<td>
Hydrogen bonding interaction in solvent</td>
</tr>
<tr>
<td colspan="2">
Solute dissociated without interactions</td>
<td colspan="2">
Reversed polarity of interactions</td>
</tr>
</table>

Table D.2 (cont'd)

 Ionic species as molecules	 Chemical reaction with water

APPENDIX E — CODEBOOK DEFINING AND DESCRIBING CODES GENERATED TO CHARACTERIZE STUDENTS' USE OF INTERACTIONS IN REPRESENTING SOLUTIONS AND THE SOLVATION PROCESS

Code definitions, clarifications, and exemplars

These codes are mutually exclusive, within *each "dissolving" and "dissolved" pane.*

ALL interactions discussed in the coding refers to interactions BETWEEN solute and solvent

Codes are first *defined and summarized,* then *exemplars are provided in the table following definitions. For clarity, coding exemplars are separated into two sections:* ***during*** *and* ***after****.*

Code names and abbreviations used throughout the codebook are shown below in Table E.1*.*

Table E.1 — Code names and abbreviations for coding representations

Code Name	Abbreviation
Off-Task	OT
No Interactions	NI
No Solute-Solvent Interactions	NSSI
Some Interactions, Incorrect Structure	NI
Incomplete Interactions	II
Complete Interactions	CI

Code Summaries

- Off-Task (OT)
    - Representations that are ambiguous or uninterpretable are coded as OT, **UNLESS** there are interactions (which would be a SI response)
    - Other examples of OT representations:
        - Not at the molecular level

        - Include ONLY solute OR solvent
        - BOTH: incorrect structure (e.g. salt as a molecule, incorrect water molecules) **AND** no interactions
        - Depictions of chemical reactions taking place (formation of covalent bonds)
        - Additionally, for during: No change between before and during

- No Interactions (NI)
    - This code must take into account the sequence from the previous pane (whether before → during OR during → after).
        - "No Interactions" means that something that was present in the previous pane is no longer intact, AND that there are no interactions present that would explain or account for how the previously associated ions/molecules became separated
        - i.e., there is/are no MECHANISM or INTERACTIONS that account for the separation

- No Solute-Solvent Interactions (NSSI)
    - The limiting factor here (between OT and NSSI representations) is presence of appropriate structures, but with NO interactions BETWEEN the solute and the solvent
    - Appropriate structures:
        - Are not necessarily complete, but components must include: Ionic lattice OR isolated ions **AND** solvent molecules
        - An INTACT solute is <u>not</u> required for "appropriate structure"
    - Interactions only <u>within</u> solute (ion-ion interactions) and/or only <u>within</u> solvent (H-bonding in water) are coded as "no interactions".

- Some Interactions, Incorrect Structure (SI)
    - Any representation that includes ***<u>EXPLICIT</u>*** interactions is, at minimum, coded as SI.
    - Examples of "Incorrect structure":
        - Lack of intact (crystalline) solute
            - Intact solute: Some of the ionic structure from the previous pane is still present. This can range from <u>a single pair of ions</u> remaining if the remaining ions are separated from each other to a <u>single ion detaching</u> from the original structure.
            - NOTE: in the first example above (single pair remaining), the rest of the ions <u>must not</u> be arranged in pairs. This would result in a code reflecting "incorrect structure" being applied.
        - Uninterpretable / ambiguous structure

        - Ionic salt in "molecules"; e.g.: individual Na-Cl representations CANNOT be coded higher than SI (i.e. cannot be coded as II or CI), regardless of other components of representation
        - For ionic representations where ions have obvious differences in size, incorrect pairing of ions with solvent (e.g.: large ion [should be Cl^- in example of NaCl] paired with δ- oxygen in water) is treated as "incorrect structure".
            - Ionic representations where ions are labeled, but are of similar sizes does <u>not</u> automatically require a SI code. The balance of the representation will then determine the appropriate code.
    - We are not differentiating between "correct" and problematic representations of interactions between solute and solvent
        - Often ambiguous representations of structure and/or interactions will imply that either the structure is incorrect or the interactions are incorrect. BOTH of these cases are coded as SI, negating the need to distinguish between the two cases.
        - **<u>However</u>**: if the interactions are clearly incorrect, or are ambiguous or occasionally inconsistent, the *highest* possible level is SI.
        - **<u>Note</u>**: If it is clear that the orientation of solute and solvent is not systematic (e.g.: every cation is spatially close to both δ+ and δ- portions of solvent or vice versa) then this would ***NOT*** be considered an interaction, and would therefore be coded in NSSI.
    - Interactions MUST be between the solute and the solvent. Interactions only within solute (ion-ion interactions) and/or only within solvent (H-bonding in water) are coded in NSSI, as previously defined.

- Incomplete Interactions (II)
    - Everything present is correct, but there are missing components.
    - During:
        - Solvent molecules are present AND are interacting with solute ions
        - Intact (crystalline) solute MUST be present
            - Intact solute: Some of the ionic structure from the previous pane is still present. This can range from <u>a single pair of ions</u> remaining if the remaining ions are separated from each other to a <u>single ion detaching</u> from the original structure.
        - There are no interactions (either implicit OR explicit) between solvent molecules and ions in the INTACT solute
        - REMEMBER: ambiguous/incorrect/occasionally inconsistent interactions cannot be coded higher than SI
    - After:
        - This is not frequently seen
        - "Incomplete" because:
            - ONLY positive OR negative ions are present and interacting with solvent molecules

            - Some solute ions are not interacting with solvent molecules
        - REMEMBER: ambiguous/incorrect/occasionally inconsistent interactions cannot be coded higher than SI

- Complete Interactions (CI)
    - Most sophisticated representation of interactions; interactions can be either EXPLICIT or IMPLICIT
    - During:
        - Ionic salt is partially dissolved
            - Intact (crystalline) solute MUST BE present
                - Intact solute: Some of the ionic structure from the previous pane is still present. This can range from <u>a single pair of ions</u> remaining if the remaining ions are separated from each other to a <u>single ion detaching</u> from the original structure.
            - Solvent molecules MUST BE interacting with intact solute
            - Isolated solute particles may also be preset
                - Solvent molecules *MUST* be interacting with "isolated" solute particles if they are present. These interactions may be either implicit or explicit, but the solvent molecules must be appropriately oriented.
    - After:
        - Ionic salt is completely dissolved
            - **ALL** ions are interacting with the appropriate part of solvent molecules (cations with δ- O, and anions with δ+ H)

Table E.2 below contains exemplars for each code, descriptions of why each exemplar has received the indicated code, and general notes for the codes as applied in this research.

Table E.2 — Code exemplars, explanations, and coding notes for coding representations

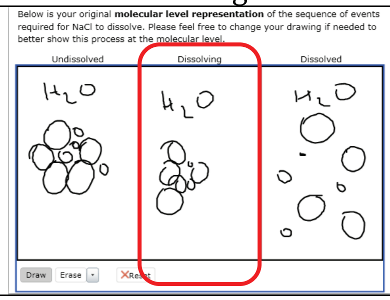
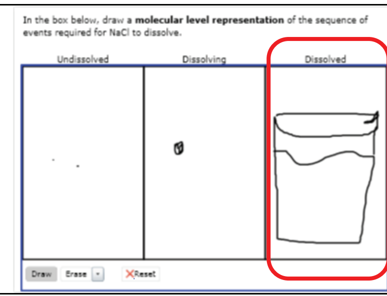
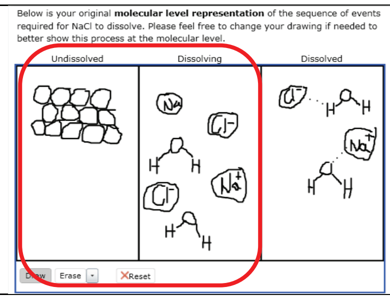
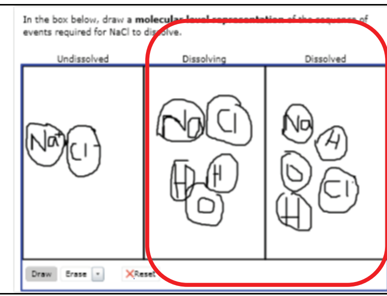
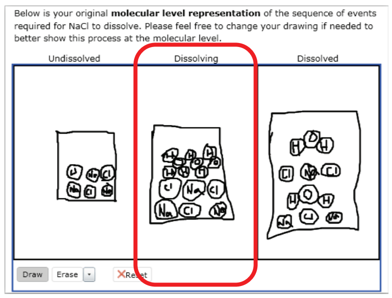
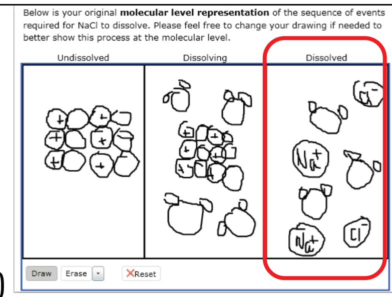
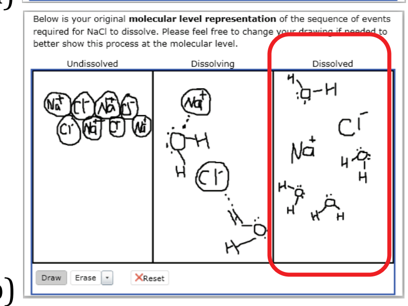
Code	During	After
Off-Task		
	Ambiguous (incorrect) structure, and no interactions	Not at the molecular level
No Interactions		
	Recall that "No Interactions apart" requires the consideration of the previous panel. The solute must be in smaller pieces, and **without** interactions that can account for how the particles became separated. There will be no interactions present in this level. In this example, there are no implicit interactions present because there appears to be no systematic arrangement of opposite charges (e.g. H is close to both Cl^- and H^+, and Cl^- is also close to both H and O), as would be required for interactions. Furthermore, the explicit interactions in the after pane (and the difference between the representations) support the conclusion that there are no interactions present in the during pane.	Same as in *during*.

Table E.2 (cont'd)

<table>
<tr><th>Code</th><th>During</th><th>After</th></tr>
<tr><td rowspan="2">No Solute-Solvent Interactions</td><td>
</td><td>(a) 

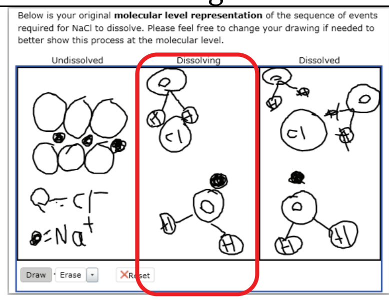
(b) 
</td></tr>
<tr><td>While the structures are difficult to interpret, there appears to be an intact solute underneath a group of water molecules. There are no (implicit) interactions here because the partially positive hydrogen (from water) is close to both Cl^- and Na^+ ions.

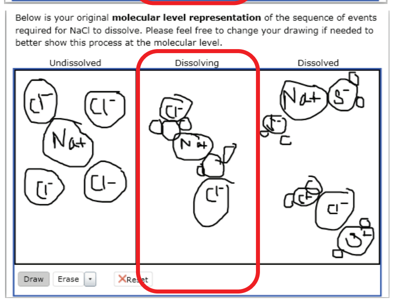
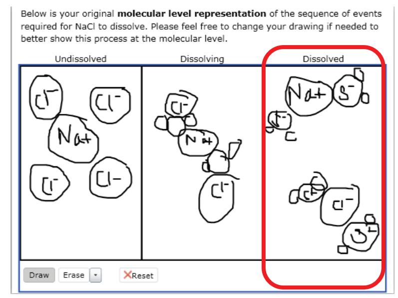
An intact solute <u>IS NOT</u> required for this level

Often NSSI during means that all of the components are present, but there are no interactions.</td><td>Example (a) is NSSI because the structures are correct, but there are no interactions present. While the two Na^+ ions are close to a water molecule, they would be interacting with oppositely charged ends of the water, so we do not consider this to be an implicit interaction.

Often NSSI after means that all components are present, and that interactions were present in the during pane that can explain the subsequent separation of the particles (see b, above). <u>Without</u> the interactions in the during pane, this would be considered "blown apart", and coded as NI.</td></tr>
</table>

Table E.2 (cont'd)

<table>
<tr><th>Code</th><th>During</th><th>After</th></tr>
<tr><td rowspan="2">Some Interactions incorrect structure</td><td>(a) 

(b) 
</td><td>
</td></tr>
<tr><td>SI requires interactions, but we are not differentiating between correct and problematic depictions of interactions.

In both (a) and (b), there are implicit interactions. There is no dashed line or other indication of an interaction. Instead the proximity of the two species implies the presence of an interaction. Even though (b) appears to have inconsistent interactions (or incorrect structures for water) it is still classified as SI because there we can infer that interactions are present due to the proximity of the solvent and solute particles.

There is no intact solute present in either example above. An intact solute is required to consider the structure "correct" for the during pane. As such, both of these are classified as SI.</td><td>In this case, either the structures must be incorrect or the interactions must be incorrect. This is because both ions are interacting with center of the solvent molecules, which implies that either the solvent molecule is not the same, or that the interactions are between species of the same charge.</td></tr>
</table>

Table E.2 (cont'd)

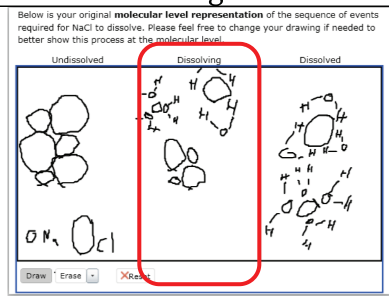
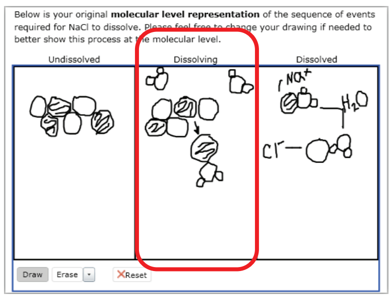
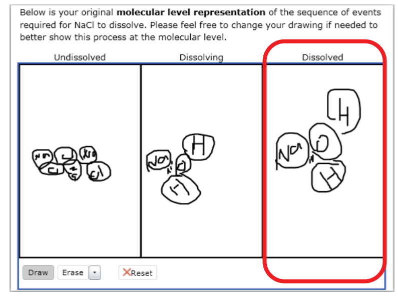
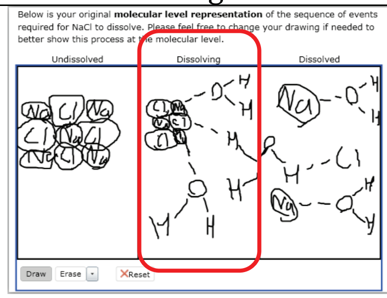
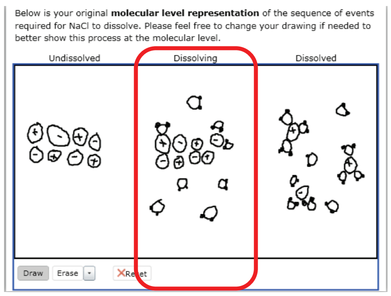
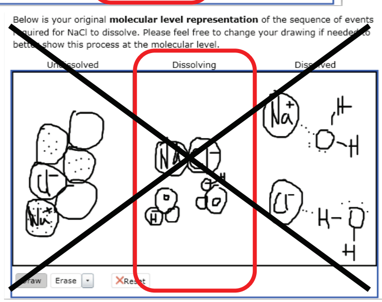
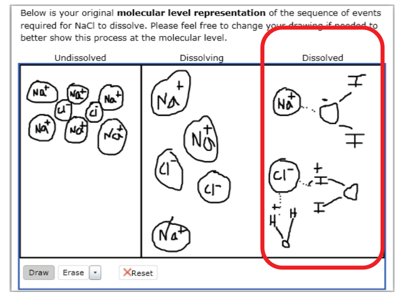
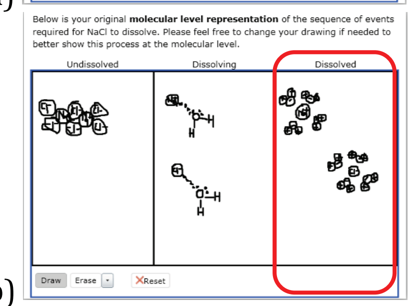
Code	During	After
Incomplete Interactions	(a)  (b) 	
	Both (a) and (b) include water molecules and an intact solute, therefore we are able to classify these as "correct" structures. The reason these are "imcomplete" interactions is because there is no interaction (either implicit or explicit) between solvent and the intact solute. While (b) may appear to have an interaction with the intact solute, it is unclear whether there was an interaction with the intact solute that caused the Na^+ ion to separate or if the ion left the solid first, and *then* established an interaction with the solvent molecule. For this reason we also classify (b) as II.	In the *after* pane, II is only (has only been) applied when the representation is correct except that only one of the ions (either cation OR anion) is depicted as being solvated. Here, the "squiggle" between sodium and water is an explicit interaction, but since there is no chloride the representation is classified as II.

Table E.2 (cont'd)

<table>
<tr><th>Code</th><th>During</th><th>After</th></tr>
<tr><td rowspan="2">Complete Interactions</td><td>(a) 

(b) 

(counter) </td><td>(a) 

(b) 
</td></tr>
<tr><td>The representation in (a) contains an intact solute, and (explicit) interactions between solvent molecules and that intact solute. Note that implicit interactions, as in (b), are also valid for CI representations.

Note the difference in (counter): the representation of NaCl is as a molecule, which we DO NOT consider to be an "intact solute". While there are implicit interactions in (counter), the lack of an intact solute means that this is classified as an incorrect structure, and therefore this is a SI representation.</td><td>For CI after, the only requirements are individual ions interacting (with correct polarity) with solvent molecules. These interactions can be either explicit (a) or implicit (b).</td></tr>
</table>

APPENDIX F — SUMMARY OF CODES GENERATED DURING DEVELOPMENT OF CODING SCHEMES TO ANALYZE STUDENT RESPONSES TO TESA

Table F.1 — Summary of all codes generated during all analysis stages of TESA coding development

Coding Scheme	Codes Developed
Initial Coding	Balance/comparison Canonical Noncanonical-forming requires Noncanonical-breaking releases Noncanonical-both Ambiguous comparison Ixns solution weaker Ixns solution stronger Canonical - nonspecific Compare rate of breaking/forming ixns Single Breaking=exothermic Breaking=endothermic Descriptive Description of heat flow Solvent/Solute attractions Because Entrogy / Gibbs Because endothermic Describe ixns formed temp system decreases, bc exothermic Water removes ions, no energy mentioned Becoming more stable Energy lost/transferred to/between ixns dissolving changes movement -> temp differential Definition of Temperature Sys temp incr, surr temp decr Dissolving is breaking ixns in NaCl

Table F.1 (cont'd)

Coding Scheme	Codes Developed
Initial Coding (continued)	Other No Answer IDK Unclear Irrelevant? Mechanism Collisions Movement / vibrations Heat Pulling/tugging
Axial Coding	Balance of forces / comparison canonical noncanonical Single force / factor canonical noncanonical Descriptive canonical noncanonical Mechanism canonical noncanonical Other / ambiguous other
Coding for Components	Collisions Balance Single Energy/temp Ixns ONLY
Coding for Energy	Coding for Energy 0 - Off-task 1 - Single Component 2 - Balance, incorrect 3 - Balance, nonspecific 4 - Balance, correct
Coding for Interactions	Present Explicit nonSpecific Absent nonIntact Solute Absent

APPENDIX G — COMPLETE CODEBOOK FOR CODING TESA RESPONSES FOR EVIDENCE OF INTERACTIONS

Prompts

Original Prompt:

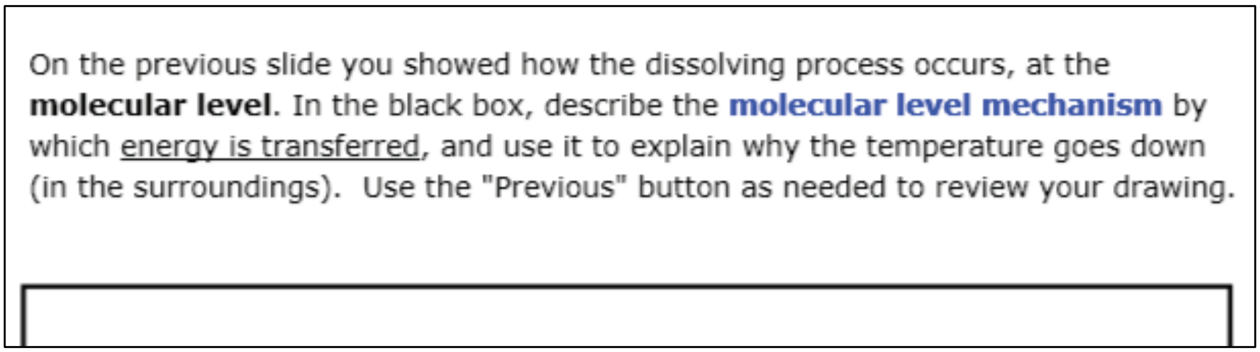


Figure G.1 — TESAv1 as administered in formative assessments

New Prompt:

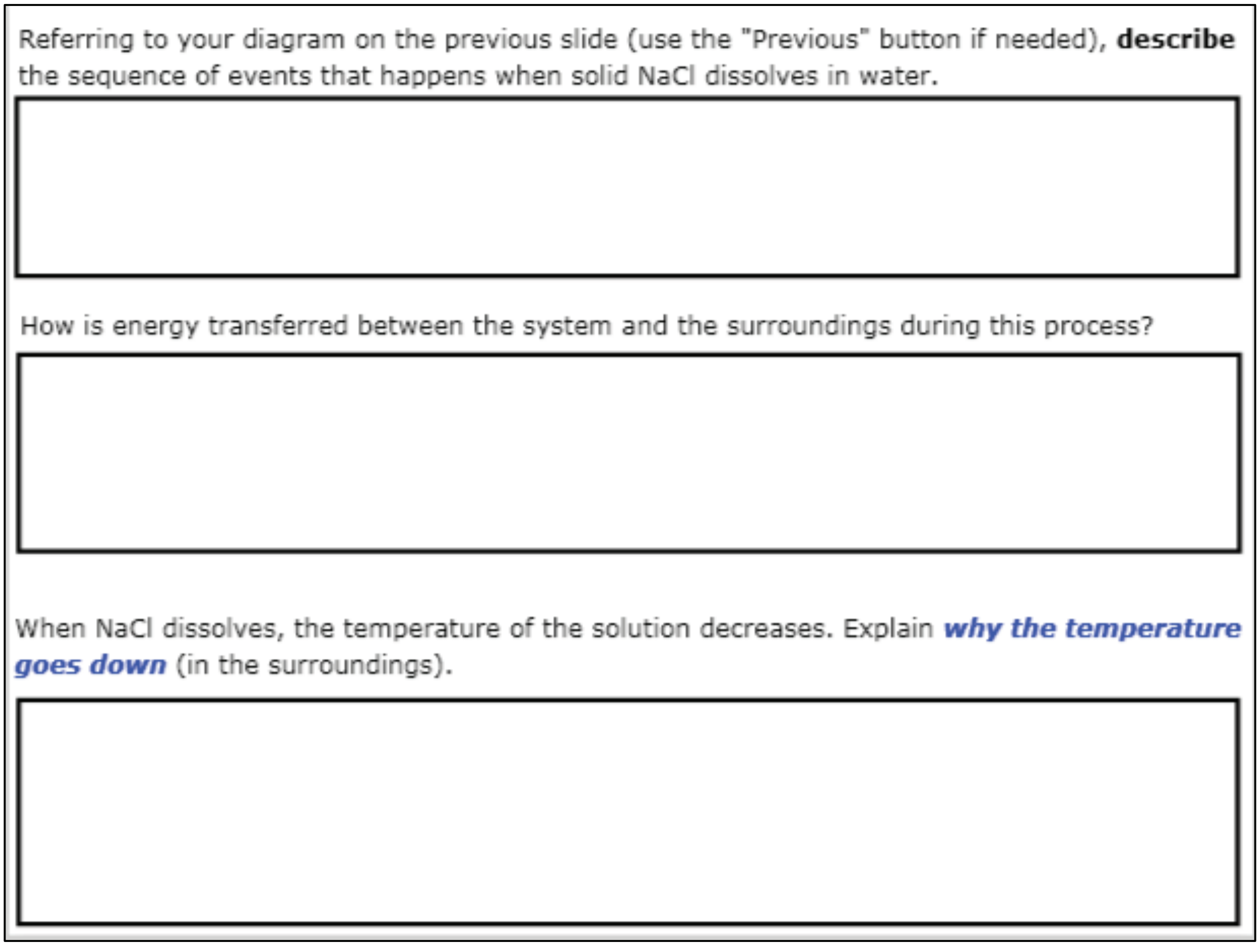


Figure G.2 — TESAfinal as administered in formative assessments

Code definitions, clarifications, and exemplars

ALL codes are mutually exclusive.

Present/Absent categories refer to interactions BETWEEN the intact solute and the solvent.

For the new prompt, anything students write, in any box is considered; the location of response is not considered when determining what code should be applied. That is, we are not only looking for components of the described interactions in certain text boxes. If components of described interactions appear at all then the code is applied.

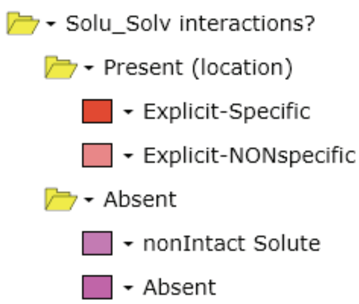


Figure G.3 — Schematic diagram showing structure of codes

For all of these codes, we are NOT analyzing correctness or accuracy of students' descriptions of the interactions that are present, only whether they are included.

<u>Present</u>

Student response refers to interactions between the solvent and an intact solute, either by explicitly talking about "interactions" or by talking about collisions.

This can be indicated by students describing concerted or simultaneous processes as indicated by "and" or "as"

Explicit-Specific

Description:

- This code is applied when student response explicitly refers to what part of the solvent interacts with what part of the intact solute

ex. "The positive charged ends of the hydrogens are attracted to the negative Cl. This interaction cleaves the Cl from the Na in a chain reaction kind of way. The negative oxygens in water attract the positive Na much like the hydrogens."

NOTE: This response explicitly mentions which ions are attracted to specifc parts of the solvent molecules. It is clear that the solute was intact before the interactions were formed because the respoonse states that the "interactions leaves the Cl from the Na"

ex. "As the NaCl enters the same space as the water the ionic bond between NaCl is broken as the polarity of the water pulls the Na to the negative O and the Cl to the positive H."

NOTE: Similar to the previous example, here the response indicates that the ionic bonding interaction is overcome "as the … water pulls the Na" apart from the chloride. Again, this response is explicit because the explanation clearly states that the sodium interacts with the oxygen while the chloride interacts with the hydrogen.

Explicit-nonSpecific

Description:

- This code is applied when student response does not specifically refer to what part of the solvent interacts with what part of the intact solute.
- Often applied when response only refers to collisions, or that the solvent interacts with the solid solute

ex. "Because H_2O polar molecules are able to overcome the NaCl ionic bonds, pulling them apart"

ex. "Water molecules will speed up and come together to remove the Cl and Na from each other. Since it sped up it required energy which the system took from the surroundings."

NOTE: because the NaCl is being "pulled apart" or "remove[d]… from each other", this is an interaction with an intact solute. These are not coded as "Explicit" because there is nothing indicating which ions are interacting with which part of the solvent molecules.

ex. "Energy is transferred through the collision of molecules bouncing into each other"

NOTE: collisions are interactions with an intact solute by definition. *HOWEVER*, single word responses such as "collisions" are <u>not</u> coded as explicitly between an intact solute and the solvent

ex. "interactions in the solid NaCl are overcome and NaCl molecules begin to dissociate from solid NaCl as they form new interactions with the H_2O molecules."

NOTE: interactions with an intact solute can be indicated in student responses by using "and" or "as" to describe a concerted or simultaneous processes

<u>Absent</u>

Student response either does not refer to interactions at all, or only talks about interactions between the solvent and isolated solvent ions. *The use of the word "absent" does not mean that interactions are absent from the response. It means that interactions between an intact solute and the solvent are absent.*

nonIntact Solute

Description:

- This code is applied when student response refers, either explicitly or implicitly, to interactions **BUT** either only refers to interaction where solute is already dissolved or where it is not obvious that the solute is still intact

ex. "When the ion-molecule bonds between the NaCl ions and the H2O molecules form out of electrostatic attraction, energy is released into the surroundings. This is known as the hydration energy and is aided by thermal motion."

NOTE: Interactions are definitely here, but referring to "NaCl ions" here makes me code this as nonIntact ("ions" implies that they have already separated). Because there is nothing explicitly telling us that these ions are still together we code this as nonIntact

Absent

Description:

- There is no reference to interactions in student's response

ex. "The heat energy transferred. When the NaCl dissoving in water, absorb the heat from surrounding. Therefore the temperature goes down."

NOTE: macroscopic level responses (usually primarily talking about heat or solute dissolving) are coded as "Absent"

ex. "The mechanism that is happening is that Na molecules are removed first and then the Cl molecules which occurs because its a alkali halide. Therefore the energy is put into the system to break these bonds, causing a drop in the temp."

NOTE: no reference to interactions even though ions are discussed

APPENDIX H — DETAILED RESULTS OF STATISTICAL TESTS COMPARING RESPONSES TO EXPLANATION AND REPRESENTATION TASKS

Table H.1 — Effect of TESA Version on interaction coding and associated chi-square statistics

			Assessment Version			Total
			Initial Prompt	First Revised TESA	Final Revised TESA	
Interaction Code	Present - Explicit	Count	0_a	8_a	22_b	30
		Expected Count	8.2	12.0	9.8	30.0
		% within Assess. Version	0.0%	8.0%	26.8%	12.0%
		Stand. Residual	-2.857	-1.155	3.876	
	Present - nonSpecific	Count	2_a	11_a	31_b	44
		Expected Count	12.0	17.6	14.4	44.0
		% within Assess. Version	2.9%	11.0%	37.8%	17.6%
		Stand. Residual	-2.881	-1.573	4.361	
	Absent - nonIntact	Count	21_a	53_b	28_a	102
		Expected Count	27.7	40.8	33.5	102.0
		% within Assess. Version	30.9%	53.0%	34.1%	40.8%
		Stand. Residual	-1.280	1.910	-.943	
	Absent - None	Count	45_a	28_b	1_c	74
		Expected Count	20.1	29.6	24.3	74.0
		% within Assess. Version	66.2%	28.0%	1.2%	29.6%
		Stand. Residual	5.544	-.294	-4.724	
Total		Count	68	100	82	250
		Expected Count	68.0	100.0	82.0	250.0
		% within Assess. Version	100.0%	100.0%	100.0%	100.0%

Chi-Square Tests

	Value	df	Asymptotic Significance (2-sided)
Pearson Chi-Square	113.629	6	<0.0005
Cramer's V	.477		<0.0005

Each subscript letter denotes a subset of Assessment Version categories whose column proportions do not differ significantly from each other at the α = .05 level. (Bonferroni corrected)

Table H.2 — Chi-square statistics testing for association between assessment type and students' use of interactions and coding summary of types of interactions observed in drawing and explanation responses to the SRA and TESAv1 in Fall 2015

Solvent-Solute Interactions Present (Collapsed Code)	Explanations	Drawings	Statistics	
Intact	19%	26%	Chi-square	3.031
nonIntact	53%	41%	*df*	2
None	28%	33%	*p*-value	0.220

Table H.3 — Results and test statistics of WSRT comparing students' use of interactions in drawing and explanation responses to the SRA and TESAv1 in Fall 2015

Ranks

		N	Mean Rank	Sum of Ranks
Explanation Interactions - Drawing Interactions	Negative Ranks	28[a]	28.41	795.50
	Positive Ranks	27[b]	27.57	744.50
	Ties	45[c]		
	Total	100		
Test Statistic	Z		-.231[d]	
	Exact. Sig. (2-tailed)		.841	
	Exact Sig. (1-tailed)		.420	

a. Explanation Interactions < Drawing Interactions

b. Explanation Interactions > Drawing Interactions

c. Explanation Interactions = Drawing Interactions

d. Based on positive ranks.

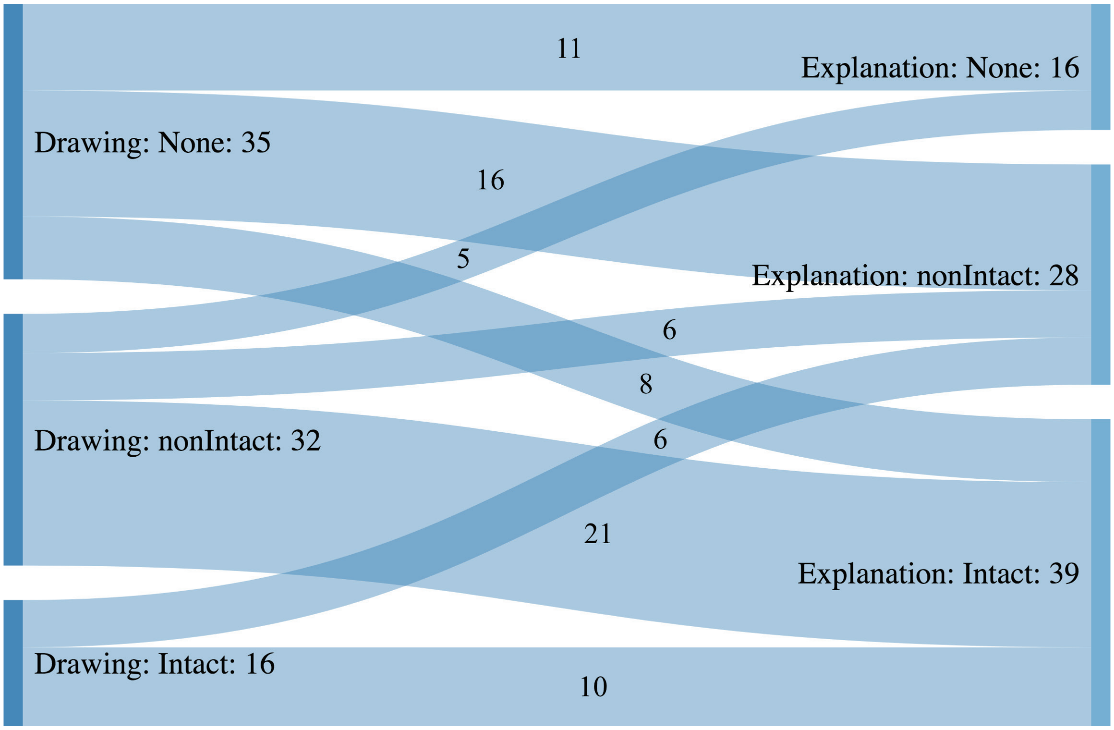


Figure H.1 —Sankey diagram displaying relationship between students' use of interactions in drawing and explanation responses to the SRA and TESAfinal in Fall 2016

Table H.4 — Results and test statistics of WSRT comparing students' use of interactions in drawing and explanation responses to the SRA and TESAfinal in Fall 2016

Ranks

		N	Mean Rank	Sum of Ranks
Explanation Interactions - Drawing Interactions	Negative Ranks	11[a]	24.50	269.50
	Positive Ranks	45[b]	29.48	1326.50
	Ties	27[c]		
	Total	83		
Test Statistic	z		-4.687[d]	
	Exact. Sig. (2-tailed)		<0.0005	
	Exact Sig. (1-tailed)		<0.0005	
	Effect size r		-0.364	

a. Explanation Interactions < Drawing Interactions

b. Explanation Interactions > Drawing Interactions

c. Explanation Interactions = Drawing Interactions

d. Based on positive ranks.

Table H.5 — Chi-square analysis of replication study of students' use of interactions in TESAfinal

			Semester		Total
			Spring 17	Fall 16	
Interaction Code	Present - Explicit	Count	22_a	20_b	42
		Standardized Residual	0.2	-0.2	
		% within Semester	26.8%	24.1%	
	Present - nonSpecific	Count	31_a	19_b	50
		Standardized Residual	1.2	-1.2	
		% within Semester	37.8%	22.9%	
	Absent - nonIntact	Count	28_a	28_a	56
		Standardized Residual	0.0	0.0	
		% within Semester	34.1%	33.7%	
	Absent - None	Count	1_a	16_b	17
		Standardized Residual	-2.6[1]	2.54	
		% within Semester	1.2%	19.3%	
Total		Count	82	83	165

Chi-Square Tests	Value	*p*-value
Pearson Chi-Square	16.205	0.001
df	3	
Cramer's V	0.313	

Each subscript letter denotes a subset of Semester categories whose column proportions do not differ significantly from each other at the .05 level.

1. Significant contributor to association between semester and students' use of interactions at the $\alpha = 0.01$ level (critical value – 2.58).

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