

Using Technology to Support the Development of Conceptual Understanding of Chemical Representations

Hsin-kai Wu, Joseph S. Krajcik, Elliot Soloway
The University of Michigan, School of Education, 610 E. University, Ann Arbor, MI 48109-1259
Tel: 734-647-4226
Email: hkwu@umich.edu, krajcik@umich.edu, soloway@umich.edu

Abstract: Many students have difficulty learning symbolic and molecular chemical representations. This study investigates how students develop their understanding of chemical representations with the aid of a visualizing tool, eChem, that allows them to build molecular models and view multiple representations simultaneously. Multiple sources of data were collected with the participation of 71 eleventh graders in a high school over a six-week period. The results of the pre- and post-tests show that students' understanding of chemical representations improved substantially ($t=13.9$, $p<.001$, effect size= 2.68). The analysis of video recordings reveals that several features in eChem helped students construct models and translate representations. Evidence also shows that high engagement students' discussions involved both visual and conceptual aspects of representations, which in turn may deepened their understandings of representations. Moreover, the findings suggest that models can serve as a vehicle for students to generate mental images, and that different types of 3D models were not used interchangeably for these students.

Keywords: visualization, science education, high school

Introduction

Students' conceptual understanding of chemical representations is a prominent area of research in chemistry education (Ben-Zvi, Eylon, & Silberstein, 1988; Gabel, 1998). For decades, researchers and chemistry educators have been discussing the three levels of representations in chemistry: macroscopic, microscopic, and symbolic levels (e.g., Gabel, Samuel, & Hunn, 1987). Chemical representations at the macroscopic level refer to observable phenomena, such as the change of matter. The microscopic chemistry refers to the nature, arrangement, and motion of molecules used to explain properties of compounds or natural phenomena. Chemistry at the symbolic level refers to the symbolic representations of atoms, molecules, and compounds, such as chemical symbols, formulas, and structures. Empirical studies (e.g. Ben-Zvi, Eylon, & Silberstein 1986, 1987) have shown that students have non-scientific conceptions at all three levels and are not able to move from one level to another. Learning microscopic and symbolic representations is especially difficult for students, since these representations are invisible and abstract while students' understandings of chemistry relies on sensory information. The teaching strategies and methods used to help students visualize chemistry at the microscopic and symbolic levels include conceptual change approaches, presentation of the historical change of a theory, using concrete models, and using technological tools (for a review: Gabel, 1998).

The visualizing tool used in the present study, eChem, is designed to play a central mediating role by allowing students to build molecular models and view multiple representations simultaneously. This study explores how high school students develop understanding of chemical representations by the use of a technological tool with similarities to professional tools, but designed for learners. Two questions guide this study: 1) Are students able to translate between two-dimensional and three-dimensional representations? If so, in what ways does eChem help students translate between representations in chemistry? 2) What learning patterns (e.g., common errors students made while making translations and constructing models, learning strategies they used to translate representations, and commonly used models for their final presentations) do students demonstrate while translating chemical representations and constructing models by using eChem? How do these patterns reveal students' development of conceptual understanding of chemical representations?

Theoretical Background

Chemical representations are the elements of chemistry language (Hoffman & Laszlo, 1991). In their ethnographic study in a chemistry laboratory, Kozma, Chin, Russell and Marx (1997) found that chemists used representations to communicate with each other and reconstructed reality and nature. They used various representations for asking questions, stating hypotheses, making claims, drawing inferences, and reaching conclusions. Being familiar with these representations and their usage in chemistry, therefore, is essential for the acquisition of expertise. Thus Kozma and Russell (1997) suggested that chemistry education should promote students to develop “representation competence.” The competence comprises a set of representational skills: the ability to see expressions with different surface features (e.g., changes in color) as representing the same principle, concept, or chemical situation, the ability to translate one representation of a chemical concept or situation into another one, and the ability to generate or select an appropriate representations to make explanation, predictions, and justification. That is, representation competence includes the skills to use a range of chemical representations to do chemistry inquiry.

However, the literature indicates that most students are unable to visualize the microscopic and symbolic representations as experts do (e.g., Ben-Zvi, Eylon, & Silberstein, 1986; Gabel et al., 1987; Kozma & Russell, 1997) and are incapable of completing the model-to-formula translations (Keig & Rubba, 1993). Various instructional and learning strategies are used to ease these learning difficulties, and the increased use of physical or computational models is striving to achieve this goal. Research supports the advantages of manipulating physical models that include helping students to visualize invisible atoms and molecules, and promoting long term understanding (Copolo & Hounshell, 1995; Gabel & Sherwood, 1980). Technological tools that integrate multiple representations provide students with opportunities to visualize chemistry and promote conceptual understanding (Kozma & Russell, 1997). Based on empirical findings of their studies, Kozma and his colleagues (Kozma et al., 1997) stated that the use of multiple, linked representations helped students understand chemical equilibrium and its related concepts.

While empirical studies assert the value of using models and technological tools for chemistry learning, however, little is understood about how models actually support students’ learning and what features of a technological tool support students to develop conceptual understanding of chemical representations. Although many professional visualizing tools have been developed for chemistry (Crouch, Holden, & Samet, 1996), none were designed for high school use. Thus, this study explores how high school students develop understanding of chemical representations by using a technological tool with similarities to professional tools, but designed for learners.

Technological Tool—eChem

The technological tool used for this study was eChem, a simplified and learner-centered version of professional visualizing tools, developed by the Center for Highly Interactive Computing in Education (hi-ce) at University of Michigan. Learner-centered design (LCD) addresses the unique needs of learners (Jackson, Krajcik, & Soloway, 1998). The principles of learner-centered design support acquisition and growth of expertise, address diversity of learners’ background, and promote and sustain motivation.

eChem guides students in three main actions—building molecules, visualizing multiple 3D models, and comparing micro- and macroscopic representations. eChem provides three tasks: *Construct*, *Visualize* and *Analyze*. In *Construct*, students can create organic molecular structures, view them from all possible angles, and manipulate them more easily than physical ball-and-stick models (see Fig. 1(A)). *Visualize* provides students with multiple views of different compounds and various representations such as ball-and-stick, wire-frame and space-fill simultaneously (see Fig. 1(B)). In *Analyze*, students can make connections between molecular models at the microscopic level (molecular structures) and their collective behaviors at the macroscopic level (chemical and physical properties).

As shown in Table 1, eChem provides various supports for chemistry learning. To support the acquisition of expertise for high school learners, eChem simplifies the periodic table to an atom palette (Fig. 1). Rather than providing the full scope of chemical bonding, constraining the scope to organic and covalent compounds simplifies the learning process, lowers the cognitive burden, and makes molecular models more understandable for novice users. Further, eChem provides only possible bonding arrangements (hybridization) to support learners to create

appropriate chemical models. Although the number of bonding arrangements is limited, complicated molecular models are still doable in eChem. For example, with the growth of expertise, students can use eChem to construct complex molecules such as glucose, DDT (DichloroDiphenyl Trichloroethane), or fatty acids. Additionally, when students choose and switch between different actions and features, eChem provides Help messages (Fig. 1) to support their learning and using process.

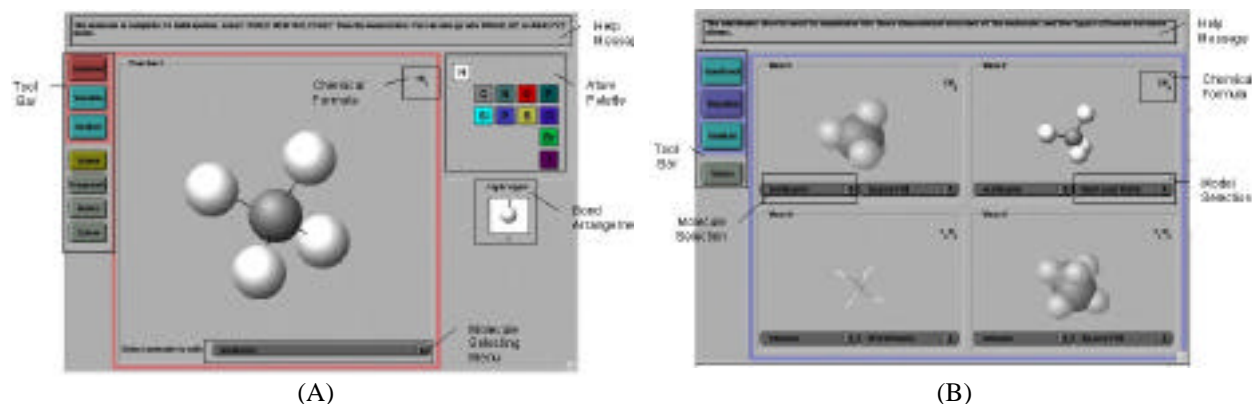


Figure 1. (A) The graphic interface of *Construct* page and (B) the graphic interface of *Visualize* page

Table 1. Learning supports provided by eChem on the three tasks.

Learning supports	Construct	Visualize	Analyze
<i>Growth of Expertise</i>			
Multiple linked representations	<ul style="list-style-type: none"> Chemical name (S), formula (S), ball-and-stick models (MI) 	<ul style="list-style-type: none"> Chemical name (S), formula (S), various 3D models (e.g., ball-and-stick, wire-frame, space-filling models)(MI) 	<ul style="list-style-type: none"> Chemical name (S), ball-and-stick model (MI), property (MA)
Reduce complexity	<ul style="list-style-type: none"> Simplified periodic table Limited bond arrangements Model rotation 	<ul style="list-style-type: none"> Select molecules Select models Model rotation 	<ul style="list-style-type: none"> Select molecules Spread sheet of structures and properties Model rotation
Explicit guidance	<ul style="list-style-type: none"> Help message 	<ul style="list-style-type: none"> Help message 	<ul style="list-style-type: none"> Help message
<i>Diversity of learners</i>			
Multiple representations	<ul style="list-style-type: none"> Chemical name (S) Chemical formula (S) Ball-and-stick model (MI) 	<ul style="list-style-type: none"> Chemical name (S) Chemical formula (S) Multiple 3D representations (MI) 	<ul style="list-style-type: none"> Chemical name (S) Ball-and-stick model (MI) Property (MA)
Non-linear path	<ul style="list-style-type: none"> Tool bar Graphic interface 	<ul style="list-style-type: none"> Tool bar Graphic interface 	<ul style="list-style-type: none"> Tool bar Graphic interface
<i>Motivation</i>			
Visual engagement	<ul style="list-style-type: none"> Graphic interface 	<ul style="list-style-type: none"> Graphic interface 	<ul style="list-style-type: none"> Graphic interface
Sustain engagement	<ul style="list-style-type: none"> Revised models Molecule database 		<ul style="list-style-type: none"> Property database

MA: macroscopic representation

MI: microscopic representation

S: symbolic representation

To address diversity of learner's background and facilitate visual engagement, eChem's visual interface supports a non-linear path to construct, visualize and analyze molecular models. Students can switch between actions and features easily by clicking buttons on the tool bar. Its multiple linked representations allow students with different learning styles to choose their preferred symbol systems (Salomon, 1979) and foster them to make connections between verbal and visual representations simultaneously (Clark & Paivio, 1991). Furthermore, compared with the built-in multimedia software which has a limited number of molecules to manipulate, eChem allows students to revise their models and create their own database of compounds over time.

Methods

Context

This study was conducted in a small public high school in an urban university town in the Midwest. The teachers in the science program worked with educational researchers from a local university to develop and implement a three-year, project-based science curriculum (Marx, Blumenfeld, Krajcik, & Soloway, 1997). Seventy-one eleventh graders in three sections participated (n=71, 35 females) and were taught by three different teachers. The students in this study had a range of ethnic backgrounds, academic abilities, and socioeconomic levels, although the majority of students were white, middle- to upper middle-class.

The use of the tool, eChem, was integrated into a six-week project called the Toxin Project. In this project, students worked in small groups and selected a known toxin to investigate from a list provided by the teachers. The driving question of this project was "Is my drinking water safe?" To answer this question, students were lectured on relevant chemical concepts, searched for information from the web, watched videos of water treatment and environmental science, carried out lab activities of solubility and water purification, built physical and eChem models, and designed webpage for final products.

From week 2 to week 4, students used three learning activities that incorporated the main actions of eChem to study hydrocarbons and alkanes (eChem I), names of alkanes (eChem II), and representations of chemistry (eChem III). The first eChem activity, tied to a lecture on covalent bonds, introduced structures and properties of organic compounds. Students constructed models of alkanes, viewed various representations simultaneously, and developed the relationship between boiling points of alkanes and the number of carbons. The second activity introduced IUPAC (International Union of Pure and Applied Chemistry) nomenclature of organic compounds, the naming rules currently used in chemistry. Students created models on eChem and followed the rules to name their models. The third activity was designed for students to visualize various two-dimensional (2D) and three-dimensional (3D) chemical representations. The 2D representations included structural formulas, condensed structural formulas, very condensed structural formulas, and chemical formulas. The 3D models constructed in this activity included the ball-and-stick, space-filling and wire-frame models. Students constructed models using eChem and ball-and-stick kits and compared differences and similarities between these two types of models.

Data Collection

Multiple sources of data were collected over a six week period. Curriculum materials, classroom videos, and field notes of classroom observations were collected to describe the implementation of the curriculum. All participants (n=71, 35 females) took pre- and post-tests. Twenty-one items were grouped into three types of conceptual understandings: 1) chemical representations, 2) chemical concepts underlying representations, and 3) connections between properties and molecular structures. Students were asked to make 2D and 3D translation, compare structural differences based on 2D structural formulas, identify types of bonding based on chemical formulas, and determine the polarity of molecules by structures. In addition, video recordings while students used eChem (process videos), students' artifacts, and interview data were collected from eighteen target students (three pairs in each section). Process videos captured activities on a computer screen and conversations of target groups. Students' artifacts included worksheets of eChem activities, models built by eChem, and webpages designed for final products. During interviews, target students were asked to predict a chemical compound's polarity and solubility, provide explanations for their predictions, represent an organic compound in various ways, manipulate molecular models mentally, and make translation between various representations.

Data Analysis

The pre- and post-tests, including multiple choice and short answer questions, evaluated students' conceptual understanding of chemical representations before and after using eChem. Process videos provided details about how target students used this visualizing tool and were coded by an analysis scheme. This scheme included students' actions of using eChem (e.g., constructing models, using visualizing feature, and analyzing properties), their actions with the use of eChem (e.g., reading aloud, writing worksheets, making comments, and discussing), and their interactions with teachers and the researcher (e.g., interventions). The amount of time students stayed in each action of eChem and the frequency students used specific features showed how various features in eChem, such as model rotation and chemical formula, helped students construct models and make translations between representations. We also examined students' levels of engagement. Engagement is defined by the amount of time students spent on discussions while using eChem. High engagement means that a student dyad spent relatively more time on thoughtful discussions containing back and forth dialogues. These discussions were transcribed and provided rich information for the investigation of how students developed understanding of molecular models.

Semi-structured interviews were conducted after students finished this project to obtain students' explanations and meanings for representations and investigate students' understanding. According to students' responses, their conceptual understanding were coded as correct/accurate, partial, and incorrect, and their ability of translation were coded as high, adequate, and low. Artifacts demonstrated students' learning progress over time. They were used to triangulate the findings of process videos and interview transcripts. For example, models and information presented on webpages were used to examine whether they were coherent with students' responses to interview questions and whether students' preferences of using a particular type of model on webpages influenced their ability to translate representations. Curriculum materials, classroom videos, and field notes of classroom observation offered evidence to examine assertions generated from other data resources. For example, students' preference of using a specific model may be influenced by the frequency of this type of model used in the class. Students' interpretation of chemical representations in interviews may be shaped by explanations that teachers provided in the class. Additionally, because process videos did not record students' physical activities, facial expressions and body languages, the data from classroom video recordings were used to complement and triangulate the findings of process video analysis.

Cases were created for each pair of focus students, and cross-case analysis was used for determining the commonalties, differences, and difficulties of translating representations and model construction. To draw conclusions, the data analysis involved generating assertions by searching the data corpus, establishing an evidentiary warrant for the assertions and verifying assertions by confirming and disconfirming evidence.

Results

A paired two-sample *t*-test for means shows statistically significant difference between means of pre- and post-tests ($t=13.9$, $p<.001$). Moreover, the effect size indicates that the average score on the post-test was more than 2.5 standard deviations greater than the average score on the pre-test (effect size=2.68). Although this study did not include a control group and the learning effects by instructions and the use of technological tool were inseparable, these results show that after this 6-week project, students acquired content knowledge at the macro and microscopic levels and were able to translate various chemical representations.

A number of themes related to students' engagement, conceptual understanding, and use of eChem emerged from the qualitative data analysis and synthesis.

Theme 1: The higher the engagement with the use of eChem, the deeper the conceptual understanding of chemical representations.

In this study, engagement is defined by the amount of time students spent on discussions while using eChem. Based on the frequency of discussions and the amount of time spent on thoughtful discussions, target student dyads are categorized as high (3 dyads), adequate (4 dyads), and low (2 dyads) engagement groups. Analysis of interviews shows that high engagement students demonstrated more accurate and correct conceptual understanding in terms of properties, structures, and underlying concepts. They were able to represent an organic molecule in various ways, describe visual differences between these representations based on the underlying

concepts such as bonding theory, identify isomers by viewing two-dimensional models, and apply underlying concepts to justify their predictions or explanations about representations.

Process videos provide data for possible explanations of how students' engagement was correlated to their conceptual understanding. When students were highly engaged in constructing, visualizing, and/or analyzing molecular models, their discussions involved the conceptual aspect of representations through which students made these representations meaningful. For example, during eChem activity one, students were asked to construct alkanes, but one pair of high students was unsure which bond arrangement of carbon was appropriate for a propane model. They clicked on the sp^2 hybrid orbital, and then found that this bond arrangement made the number of hydrogen atoms less than their prediction. It made them wonder whether the model they created was propane or not. Through building a propane model on eChem, these two students constructed (and redefined) their meanings of hydrocarbons, alkanes, and chemical bonds. During the class instruction, they acknowledged that hydrocarbon compounds were composed by carbon and hydrogen atoms. However, they did not realize how complicated chemical bonding of a hydrocarbon compound could be until they constructed this propane model. Bond arrangements provided by eChem encouraged them to consider that different bond arrangements influenced the number of hydrogen atoms attached on carbon atoms, even though the total number of bonds a carbon atom has is always the same. They also learned what counted as an alkane, which was a type of hydrocarbons with only single bonds as the compound they created, propane. Moreover, they applied their knowledge of organic chemistry and integrated the knowledge of bonding and hydrocarbons to accomplish the task. Thus, high engagement students' discussions involved the conceptual aspect of representations, such as bonding and the definition of alkanes, and that the bond arrangement feature on eChem potentially promotes students to explore various bond arrangements, search for patterns, and make chemistry bonding meaningful.

In addition to the conceptual aspect of representations, process videos show that for these high engagement students, the process of making sense of 3D models involved the visual aspect of representations. During the project, structural formulas and other 2D representations were introduced to students before they used eChem. These hand-drawing or printed 2D structures became the symbol system (Salmon, 1979) that students were familiar with. The first challenge for students to make sense of 3D view of molecules was to decode the information of bond angles and geometry of molecules that were not represented by 2D structures (Fig. 3(A)). Analysis of process videos shows that all high engagement students consciously rotated a 3D propane model from Fig. 3(B) to Fig. 3(C), because (C) looked similar to a linear 2D structural formula on paper. Through this model rotation process, the 3D model were more meaningful for students, since it shared similar visual features of the 2D one, such as relative location of hydrogen and carbon atoms and a linear carbon chain. Thus, identifying visual similarity between representations is critical for students to make sense of a novel representation.

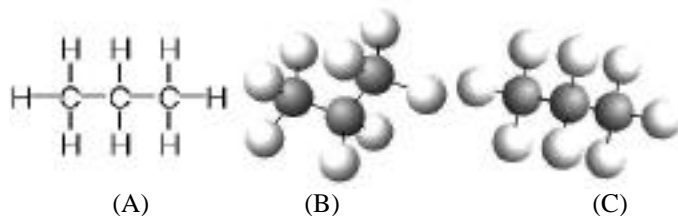


Figure 3. A 2D structural formula and 3D models of propane

Theme 2: The process of visualization involved retrieving relevant information and activating verbal and non-verbal connections in individual cognition.

To translate a chemical formula to a structural formula, some of the target students formed a mental image prior to drawing a 2D model. During the interview, in order to translate a chemical formula, C_5H_{10} , to a structural formula, one student compared this formula with the general formula of alkanes, and then transformed this formula to a mental image of what C_5H_{10} may look like.

(The interviewer shows them a chemical formula, C_5H_{10} , and asks the students translate it to a structural formula.)

S1: is it cyclopentane? (Looking at his partner, S2.)

S2: what?

S1: It's like a circle. (Using figures to make a circle.) It's not pentane, because it's C five, H twelve.
Interviewer: How do you know that?
S2: Because the formula for it, is it $2n+2$?
S1: If you get carbons, two hydrogens attach each carbon, except the ends. (Using one hand to show a linear carbon chain, and moving the other hand to locate where hydrogen atoms are around this chain.)
S1: I am thinking cyclopentane, because there aren't extra two.

The process video showed that during eChem activity I, these two students generated the general formula of alkanes by themselves based on various alkane models they built on eChem. The excerpt above indicated that they developed a conceptual linkage between formulas and structures, which included the information of symbols, structures, and mental images. They compared the unfamiliar representation, C_5H_{10} , to their prior knowledge about the reasonable number of hydrogen atoms and what an alkane should look like. They then retrieved the relevant information to make formula-to-model translation. By elaborating the idea of general formula and externalizing their mental models through verbal and non-verbal interactions with the interviewer, these students demonstrated the process of visualizing a chemical formula.

Furthermore, this excerpt reveals the interweaving nature of visualization and conceptual understanding in chemistry which could be illustrated by Paivio's dual coding theory (Clark & Paivio, 1991; Paivio, 1986). This theory explains how verbal and non-verbal representations associated with each other in individual cognition. During eChem activities, student 1 and 2 constructed a conceptual connection (connection 1) between the chemical definition of alkanes and its general formula, a visual connection (connection 2) between structural formulas and correspondent mental images, and referential connections (connection 3) between this general formula and their mental images. When they encountered the question of translating C_5H_{10} to a structural formula, all these connections were activated. Examples of connection 1 are the following comments by S1 and S2 respectively: "It's not pentane, because it's C five, H twelve." and "Because the formula for it, is it $2n+2$?" S1 externalized Connection 2 through his body language and speaking out that "If you get carbons, two hydrogens attach each carbon, except the ends." As Mayer and Anderson (1992) indicated, problem-solving transfers required both representational and referential connections. To determine that C_5H_{10} could be cyclopentane, S1 needed to activate the referential link to identify that C_5H_{10} did not fit the general formula and then triggered other possible models to solve this problem. Therefore, the process of visualizing C_5H_{10} involved making or activating the connections between verbal and non-verbal representations.

Theme 3: While models serve as a vehicle for students to construct mental images, different types of 3D models were not used interchangeably for these students.

Both physical and computational models served as a thinking vehicle for students to manipulate mentally. In response to interview questions that probed understanding of structural differences between two structural formulas, the majority of target students formed and manipulated 3D models mentally. Yet, different types of 3D models were not used interchangeably for these students. Among three types of 3D models, all target dyads chose ball-and-stick models as their 3D representations on final products. During interviews, when students were asked to identify functional groups and compare structural differences, students spent relatively less time to come up with answers if they were allowed to view the ball-and-stick models. Although the process videos showed that space-filling models were the most visually attractive to students, students did not prefer to use them to identify functional groups because bond orders were invisible in this type of models. Therefore, while wire-frame models may be too abstract by showing only carbon chains and space-filling models do not demonstrate bond orders directly, the ball and stick models were the most concrete ones for students because they convey the visible information of atoms and bond orders.

Discussions and Conclusion

The research findings of this study indicate that the visualization tool, eChem, promoted students to develop conceptual understanding of chemical representations through constructing models and viewing multiple representations. Various features of eChem provided learning supports for students to make meanings of symbolic representations. For example, bond arrangements encouraged students to rethink how different types of bonding influenced the composition of hydrocarbons. Model rotation feature assisted students to identify visual similarity between 2D and 3D models and make sense of novel 3D representations. Additionally, the chemical formula displayed on the *Construct* page helped students to identify empty bonding sites and translate a structural formula

into a 3-D model. eChem externalized the process of mental rotation and its models served as a vehicle for students to create mental image. While the empirical studies showed a modest correlation between spatial ability and learning achievement in chemistry (Carter, LaRussa, & Bodner, 1987), eChem may reduce the cognitive demanding and enable students with low spatial abilities to rotate and visualize chemical compounds.

Furthermore, the results of the study reveal that constructing visual connections between representations was as important as making conceptual connections for chemistry learning. To make sense of novel representations, students built visual connections between their prior visual experience and the new one. While the studies of novice and expert indicated that novices tend to rely on the surface features of representations to categorize representations and solve problems (Chi & Feltovich, 1981; Kozma & Russell, 1997), this study implies that chemistry learning could be built on novices' sensibility of the surface differences of features. Surface differences in representations may not be a learning barrier; rather, through the discussion and negotiation of meanings with peers, these surface or visual features could assist students to reconstruct their understanding, visualize abstract representations, and make translations. As a learning tool with multiple linked representations, eChem could provide a range of opportunities for students to interact with chemical representations, initiate group discussions, and extend students' understanding of representations.

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