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Creating Representation in Support of Chemical Reasoning to Connect Macroscopic and Submicroscopic Domains of Knowledge

Mitchell R. M. Bruce,* Alice E. Bruce, and Joseph Walter

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ABSTRACT: Chemical reasoning takes many forms. The focus in this paper is on a reasoning process that facilitates using experimental evidence to make connections between macroscopic and submicroscopic domains, which we will refer to as *creating representation*. It is a particular type of reasoning that has played a critical role in chemistry, enabling numerous scientific advancements and discoveries. Yet, the skill of creating representation is often not explicitly addressed in our introductory classrooms or laboratories. This paper outlines a process for creating and using representation that builds on other constructivist approaches but is framed in a new way to afford consistency across a continuum of novice learners to expert scientists. We illustrate how this approach is enacted in the **CORE** laboratory learning cycle (**C**hemical **O**bservations **R**epresentation **E**xperimentation), where supports are provided to help students generate ideas about representation. We also illustrate how lab reports provide opportunities for reflection, which can generate new ideas leading to revision of a representation. A comparison of **CORE** with the Atkin and Karplus learning cycle is also included to show how these different learning opportunities engage students in complementary cognitive processes to promote chemical reasoning skills.

KEYWORDS: *Introductory Chemistry, Curriculum, Analogies/Transfer, Inquiry-Based/Discovery Learning, First-Year Undergraduate/General, Problem Solving/Decision Making, Applications of Chemistry, Constructivism, Learning Theories, Chemical Education Research*

FEATURE: Chemical Education Research

■ DEVELOPING SKILLS IN SUPPORT OF CHEMICAL REASONING

The laboratory learning cycle called **CORE** (**C**hemical **O**bservations **R**epresentation **E**xperimentation)[1,2] was developed as a strategy to help students make chemical observations, generate ideas about representation, and refine those ideas through experimentation and reflection. The focus of this paper is on the process of creating representation, which underpins the **CORE** strategy. We describe how **CORE** supports the development of student skills for generating ideas about representation. This particular representation process is defined as a type of reasoning for making connections between macroscopic and submicroscopic domains using experimental evidence. We begin with a brief discussion of direct sense making and then contrast that to the inferential reasoning process required to create representation for connecting macroscopic and submicroscopic domains.

The five senses frame a common experience of the macroscopic world for most people. Historically, many chemical discoveries were made by direct "sense making" using sight, smell, hearing, taste, and touch. The Bronze Age (3300−1200 B.C.) designation originated from observations that copper mixed with about 12% tin could be cast into strong objects, especially swords, coins, and nails.[3] Around 1200 B.C., iron replaced bronze because it formed a slightly stronger material, was less prone to breaking, and reworking made it harder. Eventually observations led to changes in handling techniques and new recipes with iron, most notably adding about 2% carbon, which was observed to produce a much harder material, the alloy known as steel. Each discovery propelled further exploration, and there is no doubt that direct "sense making" has been a very powerful channel for thinking about chemistry. For many chemists, the world of descriptive chemistry has been an exceedingly important part of our education.

A new channel for chemical reasoning started to gain a foothold in the early 19th century, principally with Dalton's atomic theory, when chemists began to appreciate that information was available from a domain of knowledge beyond our senses. This new domain, which is now often called the submicroscopic, encompasses phenomena occurring at a scale that is far too small for us to directly perceive. While the direct "sense making" approach was still important, there was a shift

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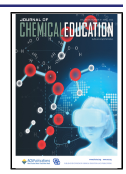

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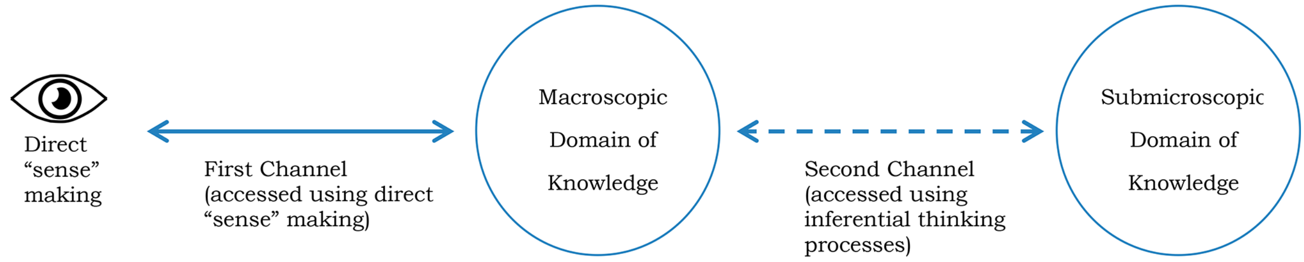

Figure 1. First channel involves knowing about the macroscopic domain of knowledge and is accessed by direct “sense” making. A second channel is established to access the submicroscopic domain of knowledge through inferential reasoning processes.

toward including chemical reasoning, which relies on inferential thinking to access the submicroscopic domain (see Figure 1).

Philosophical thinking has always probed and speculated about other domains of knowledge. What was exciting about the new atomic theory was that experimental evidence could be used as a guide for inferential thinking about the submicroscopic domain. Interest in using experimental evidence to help interpret and understand the submicroscopic domain took off over the next several centuries with the promise of new chemical insight and discoveries. This reasoning has not disappointed the world!

The second channel for chemical reasoning, i.e., the inferential thinking process that integrates experimental evidence, has resulted in breakthroughs in understanding, which reveal that the submicroscopic domain is not a miniature version of our own macroscopic world! There are several reasons why this insight is significant. First, this second channel provides access to a different domain of knowledge when reasoning about chemistry. Second, activation of this second channel necessitates learning the skill for using this type of representation, which may require ignoring macroscopic “sense making” cues. Third, we will need to modify our teaching practices to introduce new supports for helping students develop this reasoning skill.

Many words have been used to describe inferential reasoning processes for connecting macroscopic and submicroscopic domains. In this paper we refer to this process as *creating representation* and discuss our reasons for focusing on this label below. It is useful to remember that creating representation has led to many surprising, new ideas in chemistry: for example, representation describing the wave particle duality of electrons or the quantization of energy at the atomic scale. However, this inferential thinking process will be challenging for students who use direct “sense making” as the dominant reasoning method, do not understand the process of creating representation using evidence from the submicroscopic domain, or do not understand the advantages of using this type of representation. The goal of this paper is to articulate the representation creation process in experimental chemistry, which entails considering data generated in the macroscopic and submicroscopic domains of knowledge. Furthermore, we describe the **CORE** laboratory learning cycle, which offers a practical strategy to help students practice this inferential thinking skill when performing experimental lab work.

CREATING REPRESENTATION IN CORE: BUILDING ON OTHER APPROACHES TO MAKE CONNECTIONS BETWEEN MACROSCOPIC AND SUBMICROSCOPIC DOMAINS OF KNOWLEDGE

The development of **CORE** as a learning cycle was influenced by several factors that shaped our thinking about laboratory learning. These included reports and commentaries by chemists and other scientists about the importance of providing students opportunities for hands-on work accompanied by critical thinking and analysis.[4,5] We were also strongly influenced by our experience as research chemists, where our experimental investigations followed a specific sequence: making chemical observations to describe a system, reasoning to connect macroscopic and submicroscopic domains of knowledge to develop molecular level insight, and designing experiments to help refine understanding.

In 1998, supported by a FIPSE grant (US. Department of Education, P116B981469) we developed a program called InterChemNet, which allowed us to engage in pre- and post-assessment of student laboratory outcomes.[6] Initially we focused on writing lab experiments that had different laboratory learning styles.[7] Later, we developed experiments to incorporate higher levels of inquiry (i.e., above confirmation or structured inquiry).[8−10] The assessment data gathered in InterChemNet were largely used formatively to help us decide what did not work, what was promising, and what worked well. The work of Abraham and others[11−14] as well as our preliminary assessments helped us formulate an understanding of the relationship between the effectiveness of a curricular strategy and the sequence of lab activities. We began designing experiments for general chemistry students which followed a specific sequence. What emerged as we developed distinct curricular activities and supports for each part of this sequence was the **CORE** three-phase learning cycle in which the sequence of chemical **o**bservations, **r**epresentation, and **e**xperimentation became the basis of the name.

Several publications by Roald Hoffmann, Theodore L. Brown, and others, which discuss how scientists formulate connections between macroscopic and submicroscopic domains, have helped frame the issues used in the development of **CORE**. In Roald Hoffmann’s Nobel Prize acceptance speech, he highlighted the importance of using analogy for relating structures and properties of organic and inorganic molecular fragments in the isolobal analogy.[15] In another paper entitled “Representation in Chemistry”, Hoffmann describes how scientists select representations to focus on different aspects of the chemistry under investigation.[16] Hoffmann presents a series of representations of camphor and asks if each of these diagrams is true. His answer is “yes and no” to emphasize that representation is driven by what the scientist

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wants to think about or focus on. In *Making Truth: Metaphor in Science*,[17] Brown describes the important role for metaphor in guiding his ideas and understanding of the experimental systems he investigated. Brown and Hoffmann describe making connections between macroscopic and submicroscopic domains by using reasoning processes that generate ideas based on what they notice. To build this into a curricular strategy, we wanted students to generate ideas about what they notice and infer, and to reflect on the developing representation when designing experiments.

As **CORE** developed, we also were influenced by studies like *America's Lab Report*[18] and the DBER report,[19] especially those sections devoted to understanding the types of lab experiments historically used in high schools,[18] and the employment of analogical reasoning as a curricular strategy in chemistry and physics education.[19] We also became aware that the emerging **CORE** learning cycle was similar to the highly influential Atkin and Karplus learning cycle[10,20,21] but there were also some significant differences, especially in terms of the cognitive processes being accessed. Because this comparison is best described after discussing the **CORE** curricular example, a comparison between the two learning cycles is provided at the end of this paper.

CORE shares features with other curricular approaches, such as the MORE thinking frame, which, although it does not use the type of scaffolding present in the **CORE** approach, very much encourages students to refine their ideas (and models).[22,23] **CORE** also emphasizes higher levels of inquiry, by using a specific sequence of activities, and is based on the idea that there is a central importance for written reflection in chemistry reasoning.[7,9,10−13,18−26,27−32] As noted by Stacy et al., confirming understanding and applying ideas outside of the classroom can have a positive impact on overall student success in chemistry.[33] Lab reports offer students opportunities to reflect on and write about chemistry following their laboratory experience. It is also important to recognize that, even though students are asked to generate their own ideas, instructors play a key role in facilitating understanding.[34,35] Thus, professional learning experiences for the TAs are part of successful delivery of inquiry-based approaches.[36−38]

A Rose by Any Other Name...,[39] A Representation by Any Other Name

Many different words, such as "representation", "symbol", "symbolic", "analogy", "metaphor", "model", and "mental modeling", have been used in the context of connecting macroscopic and submicroscopic domains of knowledge.[17,34,35,40−49] Unfortunately, some of these words have taken on negative connotations. For example, use of analogy or metaphor has been considered by some to be a double-edged sword,[50] contentious,[51] and even labeled dangerous.[52,53] By referring to the well-known phrase "a rose by any other name would smell as sweet" in the heading of this section, we are suggesting that any of these words could be used to describe a process for connecting the macro- and submicroscopic domains. In this paper we use the word "representation" for conveying a process whereby *evidence is used to help coordinate ideas across domains*.

Representation

The word "representation" is ubiquitous in the sciences and chemistry. A search for "representation" as a topic in Web of Science comes up with over 750,000 hits, and its use in titles occurs more than 150,000 times. The Merriam-Webster definition of representation includes "an artistic likeness or image",[54] and in a chemistry context, images can be labeled as representations without further explanation. It is a word used with some familiarity by chemists, but the way it is used can be very nuanced. A list of what is considered a representation in chemistry is long and includes structures, symbols, formulas, equations, and graphs.[55] Student drawings may be solicited as representations to examine, for example, how to "draw a representation showing atoms for the combustion of methane".[56] Rau recently described representation as a process in the context of adding visual representation to text.[57] As Kozma and Russell have explained it, the "development of representational competence can be fostered by explicitly engaging students in the creation of various representations and in reflection of their meaning".[58] Chemistry representations have often been categorized based on what is seen, for example, video segments, graphs, animations, and equations, and the context of using representation is to understand what we cannot see.[58] Multiple visual representations are employed to help students gain representational competency. However, use of representation also poses some dilemmas. According to Rau, "students often learn content they do not yet understand from representations they do not yet understand".[57] This dilemma raises a critical question: how do students know what source of information to use when creating meaning of a representation?

Fisher describes how representation in chemistry involves interplay between content and design.[59] "Content" refers to the properties attributed to a representational target, while "design" is the marks, lines, etc. that one sees, which are infused together to create representation. The idea that the structure depicted in artwork is important in science has also been expressed "because scientific representation is inherently contextual".[59] Schnotz and Bannert describe a semantic process for turning a drawing into more than just perception. In this process, a propositional representation is used in model construction, thereby forming a mental model using analogical reasoning.[60] The instructions for how to use representation have been discussed in terms of what we see: a "stick model is inexplicitly non-committal with regards to possessing or not possessing atomic nuclei. The model does not preclude the possibility of representing the nuclei; chemists merely suppress them."[59] The use of models or how suppression may occur during the process of modeling is important because it suggests a central role for the individual and raises the question, what source of information is being used to decide what to include and what to ignore? These ideas are critical especially for students who are asked to process the meaning of a representation with information that may not be accessible or understood by them.

We note that descriptions for formation of representation can differ, especially in terms of the information to be considered. For example, as outlined by Schnotz and Bannert, integration of text and pictures relies on a readers' "conceptual organization" to connect propositional representations and mental models.[60] These authors do not explicitly mention the need to coordinate ideas from other domains of knowledge when forming mental models. In contrast, in Johnstone's triangle,[34] there is a direct and explicit requirement to coordinate ideas across the macroscopic and submicroscopic domains when processing representation. Coordination of ideas across domains to create representation is important in other disciplines. For example, in computer science, developing

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a "good feature representation across domains is crucial" for the process of domain adaptation, which seeks to solve a problem in the target domain by using data in the source domain.[61]

Variation of representations is also exemplified in the depiction of electrons throughout history. In the book *Representing Electrons*,[62] the author describes the history of numerous representations of the electron that were aimed at making sense of various unobservable scientific phenomena. Arabatzis notes that the variance in the representation of the electrons did not undermine its identity or existence.[62] The electron is also a good example of how submicroscopic phenomena can drive the representation process, even though the submicroscopic is usually the much less familiar domain.

Representation for Connecting Macroscopic and Submicroscopic Domains

We chose to use the word "representation" in **CORE** rather than another word to draw attention to the relationship between the process for connecting macroscopic and submicroscopic domains of knowledge within a classroom context and the scientific practices that scientists use to probe the interface between what is known and unknown. Of course, not all representation must have this purpose. A drawing of a gas cylinder, a chemical formula, and the algorithmic use of $PV = nRT$ are examples of representations as images, symbols, and text that can be used without having to connect macroscopic and submicroscopic domains. However, the emphasis in this paper is on the use of representation as a process that is exemplified by a pedagogical strategy employed in **CORE** for making connections between the macroscopic and submicroscopic domains of knowledge.

Figure 2 shows the conceptual organization for connecting macroscopic and submicroscopic domains through a process of creating representation. The process involves coordination of experimental data, ideas, and entities shown in the boxes across the domains using analogical reasoning. The meaning of the representation is developed using evidence from each domain as anchors.

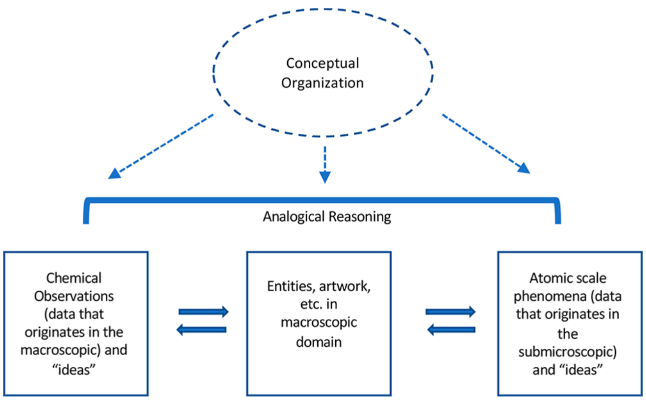

Figure 2. Conceptual organization for the representation process to connect the macroscopic and submicroscopic domains of knowledge.

The conceptual organization illustrated in Figure 2 shares some similarities with modeling[49,63−69] and the development of representational competency through the use of multiple external representations (MERs).[58,60,70−77] However, we chose to frame representation as a process that explicitly includes consideration of the submicroscopic domain rather than use, for example, a term such as "mental modeling" for several reasons. As noted by McClary and Talanquer, "a consensus view about issues such as the format of the mental models and the process involved in using them has not been reached."[78] Further, Guy-Gaytán et al. make the case that modeling instruction may not support student sense making as a result of "the tensions between viewing models as content to be learned and modeling as a scientific practice in which the end products are not known ahead of time."[79] In the **CORE** approach, macroscopic entities provided to students (e.g., paper clips, vide infra) are not initially considered as part of any representation, nor would we consider them to be models at this point. Rather, the representation process used in **CORE** emphasizes the scientific practice that considers evidence to connect macroscopic and submicroscopic domains of knowledge.

Designing experiments to probe the interface between the known and unknown is a driving force for new scientific discoveries, and the research process that creates new knowledge relies on representation to connect the domains of knowledge (macroscopic and submicroscopic). This interface between the known and unknown describes where scientists do their work. Despite the importance of this type of representation in scientific discovery, it is not often incorporated as a critical component of doing science. Rather, the "scientific method" is typically presented to students as a series of steps to solve a problem, which gives little consideration to how scientists use evidence to access the interface between what is known and unknown. Although the supposition that evidence is required to create representation is not a typical use of the word "representation", it is an appropriate use given the **CORE** framework.

In developing the **CORE** strategy to engage students in a reasoning process for creating representation, there is a strong reliance on constructivism when we ask students to generate their own ideas and understanding.[24] Literature suggests that "to reach an understanding of students' thought processes in the laboratory" students should engage in "deep processing of information", but that students have limitations in the "amount of information they can process at one time".[80] Figures and graphs are frequently used to shift the emphasis in an experiment from collection toward interpretation. But this can be a complex undertaking for students.[81] Our aim in developing **CORE** was to provide a structured, scaffolded approach, i.e., to emphasize engagement and interpretation of data without overwhelming students.

To frame this student-centered approach in **CORE**, the original work of Johnstone was also instrumental in thinking about structured supports. Johnstone's triangle is frequently cited to illustrate the connections between macroscopic, submicroscopic, and representational ideas.[34] Johnstone described how expert chemical thinking lies in the middle of the triangle, but "few of our students follow us there with any great ease." We interpreted this "middle" as involving chemical reasoning, and a desired outcome would be for students to develop these reasoning skills. The general recognition that connecting macroscopic and submicroscopic domains of knowledge is challenging for the novice learner[48,76,82−87] also supported the need for a scaffolded approach to help students develop these reasoning skills.

The **CORE** approach thus places students at the center of thinking about what is important in the chemistry under investigation and utilizes the student's own interest in

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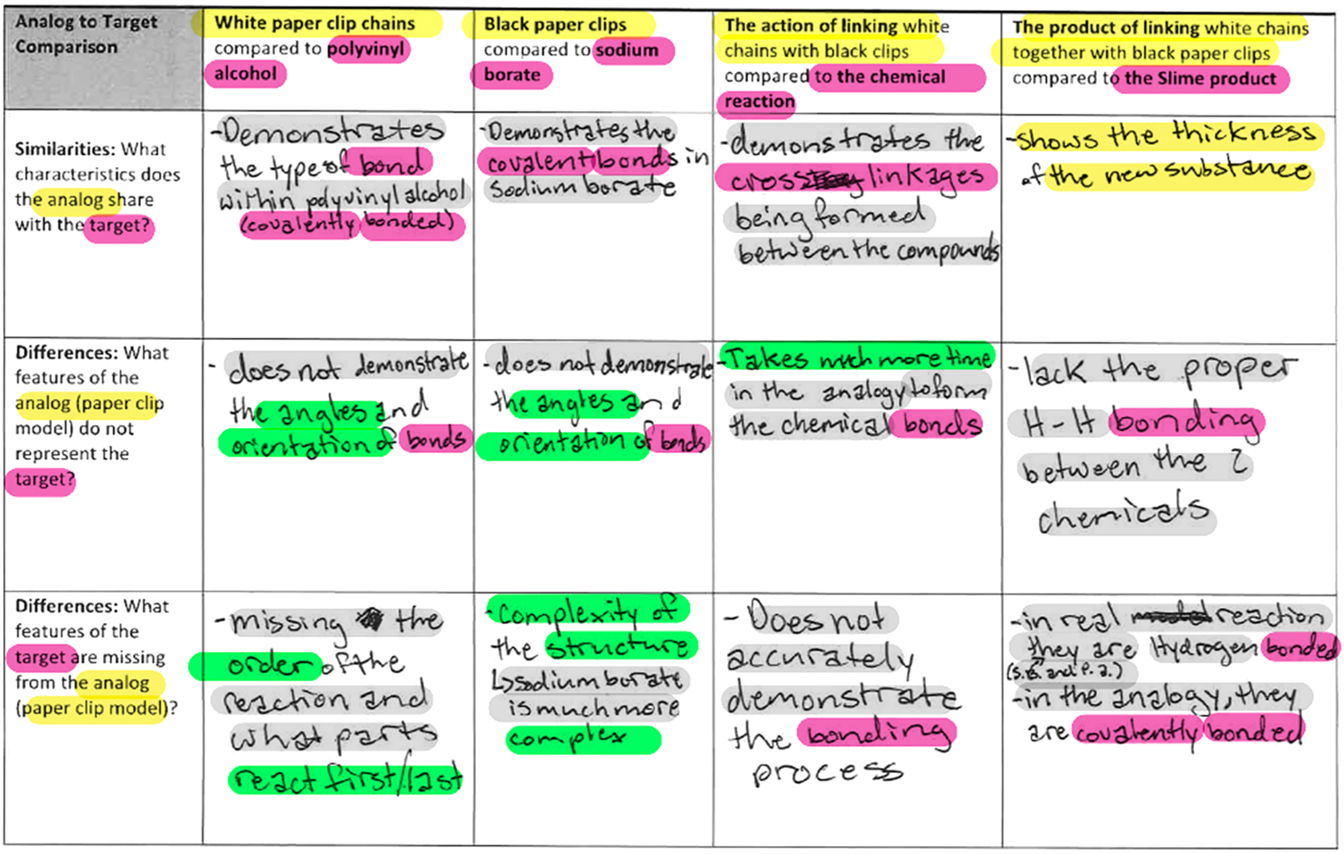

Analog to Target Comparison	White paper clip chains compared to polyvinyl alcohol	Black paper clips compared to sodium borate	The action of linking white chains with black clips compared to the chemical reaction	The product of linking white chains together with black paper clips compared to the Slime product
Similarities: What characteristics does the analog share with the target?	-Demonstrates the type of bond within polyvinyl alcohol (covalently bonded)	-Demonstrates the covalent bonds in Sodium borate	-demonstrates the cross linkages being formed between the compounds	-shows the thickness of the new substance
Differences: What features of the analog (paper clip model) do not represent the target?	- does not demonstrate the angles and orientation of bonds	-does not demonstrate the angles and orientation of bonds	-Takes much more time in the analogy to form the chemical bonds	-lack the proper H-H bonding between the 2 chemicals
Differences: What features of the target are missing from the analog (paper clip model)?	-missing the order of the reaction and what parts react first/last	-Complexity of the structure (sodium borate is much more complex	- Does not accurately demonstrate the bonding process	-in real reaction they are Hydrogen bonded (S.B. and P.A.) -in the analogy, they are covalently bonded

Figure 3. Student worksheet in **CORE** Polymers and Cross-Linking experiment. Responses are highlighted with different colors to indicate words used in macroscopic observations (in yellow; analog, model, white paper clip, chains, black, linking white chains, black paper clips, thickness, new substance); words referring to submicroscopic ideas (in magenta; target, bond, covalent, cross-linkages); words that are ambiguous, i.e., could refer to either domain (in gray; compared, poly(vinyl alcohol), sodium borate, chemical reaction, demonstrates, formed, compounds, chemical, H−H, between two chemicals, missing, reaction, parts, analogy); and ideas relating structure, sequence, and time (in green; angles, orientation, time, order, first/last, structure, complexity). We note that this worksheet has been revised from what was published previously.[1]

formulating further experimentation. Students are provided instructional materials with explicit information about the **CORE** approach to encourage metacognition.[80,88−91] In the first phase of **CORE**, to provide a common point of reference, students are guided through a series of steps to make similar chemical observations. From a constructivist perspective, we knew that at the point when students were asked to generate their own ideas, there would be some divergence in thinking, since prior knowledge and what students notice would inevitably be very different. To accommodate the process of generating individual ideas into a curricular strategy, we looked toward analogical reasoning,[40,42,92−106] structure mapping theory,[42−45,107−109] and even consideration of the importance of recognizing patterns in the development of expert thinking.[110] We distilled this down to a scaffolded process whereby students reflect on their chemical observations and employ analogical reasoning to generate their own ideas. This scaffolded process developed into the analog and target worksheet (see Figure 3). In the final phase of **CORE**, students are asked to consider their ideas and to design experiments to help refine their understandings. This is followed by an opportunity to write about the chemistry involved in the experiment (i.e., a lab report).

THE CORE STRATEGY FOR CREATING REPRESENTATION TO CONNECT MACROSCOPIC AND SUBMICROSCOPIC DOMAINS

Definition of Representation for Connecting Macroscopic and Submicroscopic Domains

To articulate the conceptual organization for the process of creating representation shown in Figure 2, we first define "representation" (as used in **CORE**), discuss the logic needed for creating meaning for a representation, and follow up with a curricular example to illustrate how it is enacted in **CORE**.

A representation for connecting macroscopic and submicroscopic domains of knowledge is any and all thinking that can be used to construct meaning between the macroscopic and submicroscopic domains. The meaning of such a representation is developed using analogical reasoning, through exploration of the similarities and differences between these nonintersecting domains. The process is inferential by nature and requires thinking about data that originate in the domains of knowledge.

The definition of representation presented here accommodates a constructivist approach, so anyone (including a novice student) may consider any and all thinking that would allow construction of a connection between domains. This definition recognizes that representation can take on a number of forms, be used in unpredictable ways, and have meanings that may not be immediately obvious. Thus, a representation

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may be used in a way that has not been used before and has the potential to lead to new insights in a similar way that disruptive technology can be innovative and change the way people think.

An essential feature of creating a representation is to engage in a process that leads to the construction of meaning across domains. A well-known, historical example comes from August Kekulé, who conceived of the image of a snake biting its own tail to describe the concept of aromaticity in benzene.[111] At the time he was thinking about this, we might assume that the image had never been used as a representation for this purpose. An image existing in our macroscopic world will not necessarily be a representation to connect domains of knowledge until the user explores similarities and differences between the domains and considers data that are relevant for both. This is a crucial point, in that the exploration process requires reflection on the similarities and differences between domains and will depend on what data are considered, what is noticed, and what connections are developed. Therefore, two people may construct different representations when considering the same idea or image. Furthermore, someone who does not engage in the representation process would see only an image. The last situation is extremely germane for students, because even if an image, such as a ball and stick model, is labeled as a representation, students will not automatically engage in chemical reasoning to connect the macroscopic (what they can see) with the submicroscopic (e.g., volume of atoms, location of electrons).[83−87,112] This suggests that, without a strategy to help students learn about the process, many students will not be capable of understanding how to develop ideas into representations.

Creating Meaning of a Representation: The Process for Connecting Macroscopic and Submicroscopic Domains of Knowledge

Creating representation for the purpose of connecting macroscopic and submicroscopic domains of knowledge as outlined above involves considering data that are relevant in both domains and exploring the similarities and differences between these nonintersecting domains. The logic we utilize to accomplish this in **CORE** is analogical reasoning. There are several learning strategies, which emphasize examining the similarities and differences when constructing connections between domains of knowledge, i.e., the teaching with analogies model and structure mapping theory.[42,96,113] According to Merriam-Webster, "analogical" is defined as "of, related to, or based on analogy" and an analogy is "a comparison of two otherwise unlike things based on resemblance of a particular aspect" and "resemblance in some particulars between things otherwise unlike".[114] Analogical reasoning allows comparisons of ideas across domains, utilizing data available in both domains. This can result in coordination of thinking across domains. A virtue of this approach is that, as information is added or modified, the meaning of a representation that aims to connect macroscopic and submicroscopic domains of knowledge can change to accommodate new thinking and data.

To illustrate how a representation process to connect macroscopic and submicroscopic domains of knowledge is a useful skill in the context of experimental chemistry, let us consider a well-accepted "content knowledge" explanation for why sodium explodes when tossed into water. The explanation that has appeared in textbooks for decades is that "this vigorous behaviour results from heat release, steam formation and ignition of the hydrogen gas that is produced".[115] Furthermore, a balanced chemical equation can be used to illustrate how the exothermic production of hydrogen gas can result in the gas being heated to a high temperature, followed by explosion. The "textbook" explanation can be considered entirely a macromodel or macrorepresentation (and not connected in any way to the submicroscopic domain). However, consider the possibility that there are submicroscopic phenomena that are not accounted for in the textbook explanation. In that case, scientists who are skilled at creating representation by using evidence to connect macroscopic and submicroscopic domains are in a better position to develop new understanding.

This is the exact situation that Mason et al. found themselves in.[115] They noted that there appeared to be information that was missing and/or contradictory to the textbook explanation. Specifically, the "textbook" explanation was not satisfactory because they reasoned that a heterogeneous process in which the reaction only occurred at the interface would need an efficient mixing of the reactants to lead to explosion. However, they did not see how such a mixing between the macroscopically heterogeneous alkali metal and water could be achieved. Further, production of steam and hydrogen gas at the interface between water and metal should create a vapor layer that would passivate the surface inhibiting the reaction. In other words, the textbook explanation was insufficient to understand the submicroscopic phenomena responsible for the macroscopic observation (i.e., explosion).

This led Mason et al. to propose additional experiments to generate new ideas about how to connect the macroscopic observations and submicroscopic phenomena. In one set of experiments, they used a high-speed camera to closely examine what happens when individual drops of sodium hit water. These results revealed submillisecond formation of metal spikes protruding from the drop. Next, they explored what was happening on the picosecond time scale, by performing molecular dynamic simulations. These calculations suggested rapid migration of electrons on the picosecond time scale. Their investigation led to a new set of ideas that they used to connect what was seen (in the macroscopic domain) to phenomena that were occurring at the atomic scale (submicroscopic domain). They describe their new macroscopic and submicroscopic understanding this way: a Coulombic explosion caused by massive charging of the surface with fast migration of electrons into water, all which "precedes and actually enables the notoriously explosive alkali metal-water reaction". Thus, new information about the explosive reaction of sodium in water was aided by considering limitations in the current understanding that ultimately led to experiments, which provided a more complete understanding of the connection between submicroscopic and macroscopic domains of knowledge.

We have included this example to suggest that learning how to create meaning of a representation to connect macroscopic and submicroscopic domains is a valuable skill for chemistry students. One of the great advantages of developing this skill is that as new "content knowledge" is incorporated into their existing ideas, students would have the ability to revise their thinking of representation by using the same process that was used to create their representation. The **CORE** approach can then be seen as part of a strategy to facilitate development of this skill. It is also important to note that, in **CORE**, a key application of analogical reasoning occurs when a macroscopic

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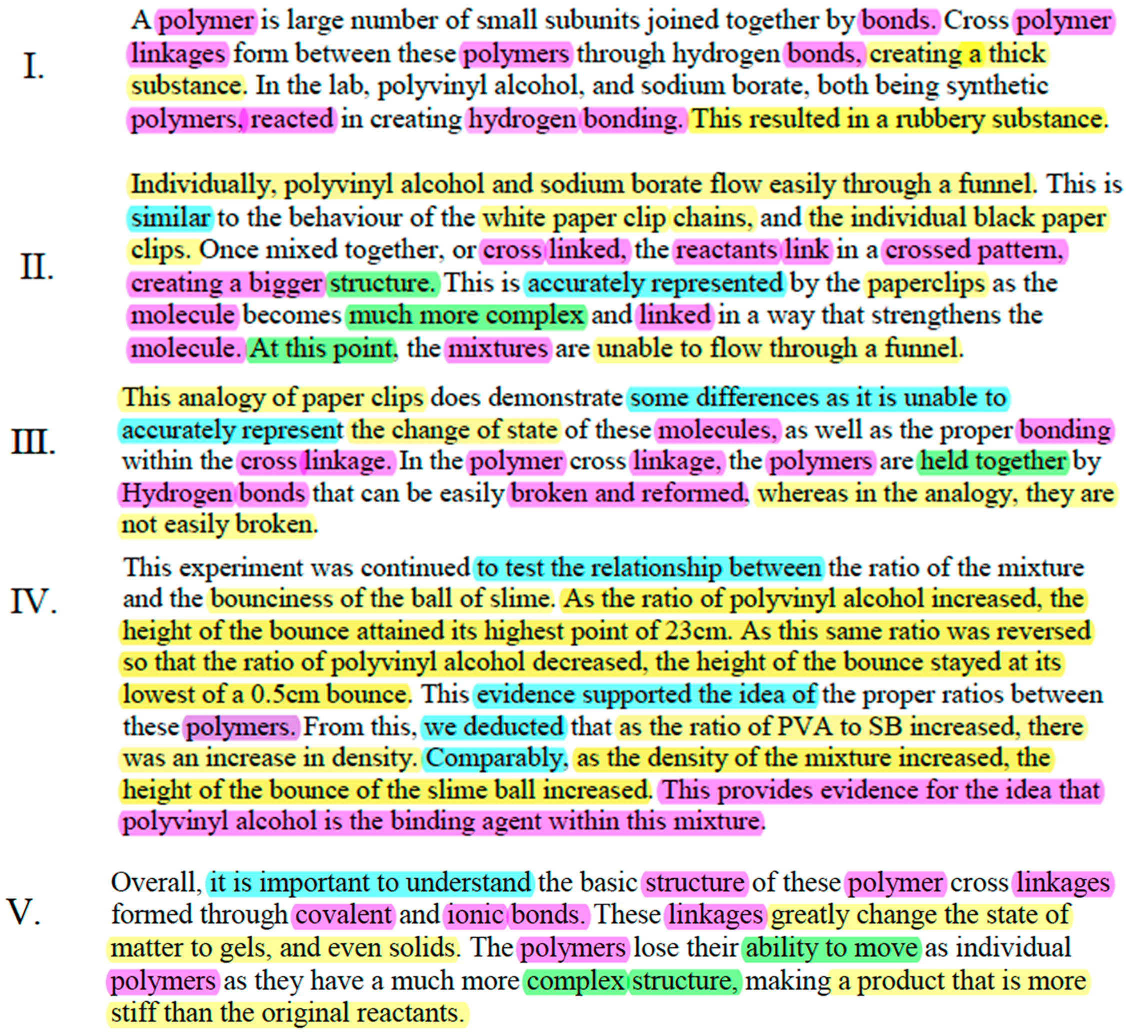
I. A polymer is large number of small subunits joined together by bonds. Cross polymer linkages form between these polymers through hydrogen bonds, creating a thick substance. In the lab, polyvinyl alcohol, and sodium borate, both being synthetic polymers, reacted in creating hydrogen bonding. This resulted in a rubbery substance.

II. Individually, polyvinyl alcohol and sodium borate flow easily through a funnel. This is similar to the behaviour of the white paper clip chains, and the individual black paper clips. Once mixed together, or cross linked, the reactants link in a crossed pattern, creating a bigger structure. This is accurately represented by the paperclips as the molecule becomes much more complex and linked in a way that strengthens the molecule. At this point, the mixtures are unable to flow through a funnel.

III. This analogy of paper clips does demonstrate some differences as it is unable to accurately represent the change of state of these molecules, as well as the proper bonding within the cross linkage. In the polymer cross linkage, the polymers are held together by Hydrogen bonds that can be easily broken and reformed, whereas in the analogy, they are not easily broken.

IV. This experiment was continued to test the relationship between the ratio of the mixture and the bounciness of the ball of slime. As the ratio of polyvinyl alcohol increased, the height of the bounce attained its highest point of 23cm. As this same ratio was reversed so that the ratio of polyvinyl alcohol decreased, the height of the bounce stayed at its lowest of a 0.5cm bounce. This evidence supported the idea of the proper ratios between these polymers. From this, we deducted that as the ratio of PVA to SB increased, there was an increase in density. Comparably, as the density of the mixture increased, the height of the bounce of the slime ball increased. This provides evidence for the idea that polyvinyl alcohol is the binding agent within this mixture.

V. Overall, it is important to understand the basic structure of these polymer cross linkages formed through covalent and ionic bonds. These linkages greatly change the state of matter to gels, and even solids. The polymers lose their ability to move as individual polymers as they have a much more complex structure, making a product that is more stiff than the original reactants.

Figure 4. Sequential paragraphs of the analysis section in a **CORE** Polymers and Cross-Linking lab report. The color coding includes words highlighted in yellow for the macroscopic domain; words highlighted in magenta for submicroscopic ideas; words highlighted in green for ideas relating to structure, sequence, and time; and words highlighted in cyan for logic involving similarities, differences, comparisons, emphasis, and deduction.

entity such as a figure, object, equation, or something that can be directly "sensed" is used as part of the process of creating representation. Skillful use of analogical reasoning can result in the identification of common features (i.e., similarities) and also appreciation of the limitations to understand the boundaries of the representation. As a consequence of recognizing the limitations of a representation (for connecting macroscopic and submicroscopic domains), some of the "sense making" cues featured in the entity may need to be ignored. This is a dynamic reasoning process that can generate growth of understanding over time. Thus, for a novice student, we may expect some missteps—but just as learning to ride a bicycle often involves missteps, the ultimate goal can still be reached.

The CORE Learning Cycle: A Curricular Example of the Support for Generating Ideas about Representation

CORE is a three-phase learning cycle in which students make chemical observations in the lab in phase 1, explore a representation in phase 2, and extend the representation with further experimentation in phase 3.[1,2] In this section, we focus on phase 2 and examine a student's responses on a worksheet, which is designed to support students in generating ideas about representation. This is followed by an examination of the same student's lab report to illustrate how these ideas can be extended to formulate and refine the representation.

In phase 1 of the **CORE** Polymers and Cross-Linking lab experiment, students conduct a series of chemical observations about the physical properties before and after mixing 0.4% solutions of sodium borate and poly(vinyl alcohol). In phase 2, students use paper clips and a powder funnel to enact parallel activities to help understand the chemistry explored in phase 1. Students then fill out a worksheet to compare the similarities and differences between the macroscopic (analog) and submicroscopic (target) domains. Figure 3 shows a student's worksheet (collected in an introductory general chemistry lab course), along with some colored highlighting to illustrate patterns and trends in the responses. Words used in reference to the macroscopic domain are highlighted in yellow, e.g., "shows the thickness"; words used in reference to the submicroscopic domain are highlighted in magenta, e.g., "bond"; and more neutral words, where the domain being referred to is ambiguous, are highlighted in gray, e.g., "sodium borate". For the purposes of identifying the scaffolding incorporated in the row and column headings, we have highlighted words to indicate their respective domains used in

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the comparison (i.e., analog to target: macroscopic to submicroscopic). We have also highlighted words in green that are important for understanding causality in chemical phenomenon, e.g., structure, complexity, sequence, and time. The colors are not meant to provide a research-based analysis but rather to illustrate the supports in the worksheet as well as the different types of ideas this student has generated. It is important to note that the student example is an illustration, and not intrinsically a presentation of research. A separate paper is planned where we use qualitative content knowledge and structure mapping theory to analyze numerous examples in order to build more comprehensive insight.[1,42,116,117]

The worksheet contains 12 different comparisons. For example, in the box that intersects with the row starting with "Similarities..." and the column heading with "The action of linking...", the student writes "demonstrates the cross linkages being formed between the compounds". The words "analog" and "The action of linking chains with black clips" in the column and row headings of the worksheet are part of the supports for thinking about the macroscopic domain, while "target" and the "chemical reaction" are part of the supports for reflecting on the submicroscopic domain. The supports appear to have been integrated into this student's ideas. Thus, the action of linking chains with black clips compared to the chemical reaction "demonstrates the cross linkages being formed between the compounds".

The worksheet provides time on task to generate ideas about a chemical phenomenon. Without making any specific claims about the nature of this student's representation, there is clear evidence that this student is generating a diverse set of ideas, which *can be used to construct meaning between the macroscopic and submicroscopic domains*, i.e., the beginning part of the representation process. To continue the process, students are asked in phase 3 to design and then carry out experiments that could be used to refine their understanding of representation. The same student from the example above devised experiments described in an experimental design worksheet (not shown) to systematically vary the ratio of PVA and sodium borate to test the bounciness of slime (in centimeters), dropping the slime from a height of 1 m, and measuring the mass, volume, and density of each piece tested. The student's additional observations were also captured in the experimental design worksheet: "as the ratio of sodium borate increased the density decreased". This example illustrates how further experimentation can generate additional data that are available in both domains, which can then be used for making further refinement of the representation.

Curricular Example of a CORE Lab Report: Using Representation in Chemical Explanations

Figure 4 shows sequential paragraphs extracted from the analysis section of a lab report submitted by the student whose worksheet is shown in Figure 3. A lab report template was provided to students to help them with formatting. There was also a rubric for the lab report that included several prompts for formulating representations, such as, "Discuss the phenomena at both the submicroscopic (molecular) level and macroscopic (visible to your eyes) level. Use the analogical model to further develop your explanations of results and underlying chemical concepts in your discussion."

Similar to the process for analysis of the worksheet, words in the lab report are highlighted to illustrate patterns and trends. Because there is more context in the report than in the worksheet, it is possible to assign words which were previously characterized as neutral or ambiguous to a domain. Ideas relating to structure, sequence, and time are again highlighted in green. A new category has been added using the color cyan to highlight words related to reasoning that draw similarities, point out differences, make comparisons, provide emphasis, or use deduction. Please note the purpose of assigning words to a specific domain is not to claim that we know precisely what the student is thinking; we acknowledge that this is an inherently individual activity. The purpose is to illustrate *how ideas between domains can be connected*.

In the first paragraph of the lab report, shown in Figure 4, the student considers evidence from lab work. Noteworthy is reasoning that connects ideas about what might be occurring at the atomic scale (e.g., "polymer linkages") with macroscopic physical properties (e.g., "a rubbery substance").

The second paragraph revisits phase 1, where macroscopic substances (i.e., poly(vinyl alcohol) and sodium borate) were observed to flow easily through a funnel. After mixing the two reagents, the student describes what is occurring at the submicroscopic level (i.e., "the reactants link" and "bigger structure"). The student also makes comparisons across domains ("similar", "accurately represented"). Finally, at the end of the paragraph, the student returns to reflecting on macroscopic properties (i.e., "unable to flow through a funnel").

The third paragraph contains ideas about the boundaries of the representation (i.e., "some differences" and "unable to accurately represent"). The student articulates ideas that span reasoning about what is occurring at the atomic scale (e.g., "cross linkage"), ideas about structure (e.g., "held together"), and the dynamic nature of the chemical interactions (e.g., "broken and reformed"). The paragraph concludes with macroscopic observations about the analog, describing the connections between paper clips as more robust (e.g., "in the analogy, they are not easily broken").

The fourth paragraph considers results of further experimentation from phase 3, where the student varied the ratio of reactants to investigate the influence on the physical properties of the mixture. Although much of the paragraph describes macroscopic, experimental results, the student's interpretation at the end seems to connect the macroscopic observational frame (i.e., density and the resulting bounciness) to structural changes at the atomic scale (i.e., "the binding agent within this mixture"). In the last paragraph, an emphasis is placed on ideas that originate from the other paragraphs to explain the structure−property relationships which are responsible for the changes in state.

In the worksheet and lab report, this student expresses several ideas that may be incorrect or at the very least may require further interpretation. For example, when asked to discuss features of the analog that do not represent the target, the student instead mentions features that belong to the target (first column, middle row: "does not demonstrate the angles and orientation of bonds"). Nevertheless, the student appears to be thinking across the domains to focus on differences that exist. In the fourth paragraph of the lab report, the student refers to poly(vinyl alcohol) as the "binding agent". Although this is not technically correct (sodium borate is the cross-linker in this system), the student notes that when they increased the poly(vinyl alcohol) to sodium borate ratio, there was an increase in density. This statement follows the evidence that perhaps an increase in PVA *caused this* result. This is not

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Table 1. Comparison between the Atkin and Karplus/EIA Learning Cycle and the Chemical Observation, Representation, Experimentation (CORE) Learning Cycle

	Atkin and Karplus/EIA Learning Cycle	**CORE** Learning Cycle
Preactivity	Review introductory materials	Review introductory materials
Phase 1	Exploration: chemical observations that focus on phenomenological views of chemistry	Chemical Observation: phenomenological view is considered along with open-ended questions to think about the chemistry at the molecular level
Phase 2	Invent: focus on "inventing concepts" and variable relationships by deriving them using observations and data	Representation: focus on "construction of a representation" by examining the similarities and differences of the different domains
Phase 3	Apply: focus on application of invented concept	Experimentation: focus on the design of experiments supported by representation with an opportunity to refine the representation

uncommon in science, where experimental results lead to the need for further experimentation to understand a phenomenon. It does not take away from the fact that this student was carefully using evidence to justify ideas. Without claiming to know precisely what representation this student had in mind, or to label it as right or wrong, this example illustrates how an *individual student used experimental evidence to generate ideas* and *create representation* to reason about chemistry by considering both domains of knowledge.

Engaging students in their initial ideas has been noted as critical for students' abilities to grasp new concepts.[118] Cognitive analogical reasoning studies have suggested that "people need not have learned something perfectly when they first encounter it—they may be capable of retrieving useful prior knowledge by developing their current understanding" and, as a consequence, "gains in knowledge can propagate not only forward in transfer but backwards to illuminate prior knowledge".[44] In **CORE**, the strategy rests on the idea that, by employing analogical reasoning, students may be able to repair understanding going forward.[44]

■ CORE VERSUS THE ATKIN AND KARPLUS LEARNING CYCLE

Atkin and Karplus Learning Cycle

In 1962, Atkin and Karplus published a paper entitled "Discovery or Invention?",[21] outlining a learning cycle that had a goal of mirroring scientific thinking to help students analyze scientific phenomenon. The clientele for the Atkin and Karplus learning cycle were elementary school children, and activities were designed to employ objects such as blocks, licorice, dowel sticks, clay, and crackers.[20] The origins of this learning cycle appear to be influenced by the constructivist ideas of Jean Piaget, who interacted with Karplus in 1961 about how children form ideas about scientific concepts.[119] One important strategy for using classroom objects to illustrate scientific phenomena was to emphasize the objects' properties rather than their common use. In this way, students were asked to analyze data that could be observed. For example, in an activity for first graders about the concept of matter, students explored what happens to a cracker when it is crumbled. Although the crumbs have a very different appearance, they are still made up of the same material as the whole cracker. A follow-up activity with a scale, to measure the mass before and after crumbling the cracker, generated data for investigating the concept of conservation of matter. In this way, each learner's progression would involve observation of a phenomenon (explore), thinking about concepts such as that whole and crumbled crackers are made up of the same substance (a type of invention that can be guided by the elementary school teacher), and then a phase involving testing, which can be used to reinforce or extend a concept (apply).

These early studies were followed by the creation of the Science Curriculum Improvement Study, a project supported by the National Science Foundation from 1963 through the mid-1970s (Award No. 6300019). Many of these lessons became exemplars of how to help students engage and build understanding of scientific concepts. A separate study of elementary students also suggested that three to four experiences with a new science idea may be needed before it is committed to long-term memory.[120,121] In many ways, these early developers can be seen as the forerunners of the NGSS standards, which are being implemented in our new century.[122] The continued need to focus on lessons like these, however, is still evident today when assessment of student performance from the AAAS Project 2061 (https://www.aaas.org/programs/project-2061/assessment-resources) shows that significant numbers of sixth to eighth grade students still find certain questions about conservation of matter very difficult.

EIA Learning Cycle

The Atkin and Karplus learning cycle was recast as the EIA (*E*xploration, *I*nvention, and *A*pplication) learning cycle for applications in high school and college chemistry courses. Two exemplars of this approach include (1) inquiry-based laboratory experiments of Abraham and Pavelich[123,124] and (2) POGIL (*P*rocess *O*riented *G*uided *I*nquiry *L*earning) classroom activities.[125]

EIA chemistry lab experiments developed by Abraham and Pavelich appeared in a laboratory manual entitled *Inquiries into Chemistry*.[123] Each chemistry experiment involved an exploration phase to collect and analyze data (exploration), a phase that formulated conclusions and/or interpretation (invention), and a third phase involving open-inquiry experiments (application). A key part of the laboratory experience comes in the second phase when the student and/or teacher derives a concept from the phenomena observed in the first phase. We note that, in the original Atkin and Karplus learning cycle, there was a central role for teachers in the invention stage, while in this EIA version it is left as an option. Research by Renner and Abraham demonstrated that the order of the EIA learning cycle plays a critical role in the extent of success.[11−13] The importance of the sequence of the EIA learning cycle has also been elaborated, analyzed, and extended in the 5E model of engagement, exploration, explanation, elaboration, and evaluation.[14]

Comparing Atkin and Karplus/EIA and CORE Approaches

The success of the Atkin and Karplus and EIA learning cycle approaches illustrates the power of an ordered sequence of activities for helping students coordinate and understand scientific concepts.[11] While we note that there is no limitation, per se, as to what goes into each of these phases, in practice the "invention" of a concept occurs from directly observable phenomena, as illustrated in the example of whole versus

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crumbled crackers in the elementary school activity. Further, these approaches can include analysis of real data, which contains experimental variation, as an important exercise in a student-centered experimental environment. For example, in the Atkin and Karplus investigation with crackers, the concept of variation in data could be introduced when students repeat the mass measurements and find slightly different masses. The conversation could then focus on the variability of taking measurements (e.g., uncertainty in measurement). The Atkin and Karplus/EIA learning cycle places an emphasis on helping students analyze concepts scientifically. However, this approach does not specifically include any scaffolding for supporting the creation of representation to make macroscopic-to-submicroscopic connections.

A comparison between the Atkin and Karplus/EIA and **CORE** learning cycles is outlined in Table 1 and reveals many similarities for what students are asked to do: review introductory materials (preactivity), investigate phenomena (phase 1), formulate explanations based on data (phase 2), and extend the activity (phase 3). While students trace similar paths, differences emerge in what students are asked to reason about in phase 2. This difference comes about as a natural consequence of the different foci in phase 3. Thus, in the Atkin and Karplus/EIA approach, students examine a relationship involving macroscopic phenomena to invent a concept and then apply their understanding of the phenomena. In **CORE**, students reason about what is occurring at the atomic scale (e.g., particulate level) through developing and constructing representation, to explain and refine understanding during phase 3 experimentation. We would argue that the skills emphasized by both approaches are needed by our students and the two learning cycles are complementary in helping students develop chemical reasoning.

CONCLUDING REMARKS

We have described the vital importance for transitioning novice students from reasoning practices dominated by direct "sense making" to those that include the creation of representation to connect macroscopic and submicroscopic domains of knowledge. To help in this effort, we present a frame of reference for creating representation, which is formulated in a manner that is accessible for novice students and is compatible with expert thinking. We illustrate how the frame for representation is enacted in the **CORE** approach, whereby students can generate ideas that can be utilized in developing a representation. This inferential reasoning process could allow students to consider new information that may alter or refine the representation.

The **CORE** learning cycle offers one approach for how students can be supported in their use of analogical reasoning for creating, utilizing, and refining representation. Comparison of the **CORE** learning cycle with the Atkin and Karplus/EIA learning cycle reveals some similarities and some significant differences in the reasoning strategy, especially in phase 2. These differences are germane to introductory students, who are often faced with being asked to consider the submicroscopic ideas in classroom and laboratory settings but may not be afforded curricular supports to be successful. The different conceptual thinking processes emphasized by the Atkin and Karplus and **CORE** learning cycles makes them complementary and synergistic approaches, which could be used side by side to help students develop a more diverse set of chemical reasoning skills for understanding chemistry.

Finally, our motivation for discussing this topic is to provide a basis to activate students more fully toward the thinking practices chemists use to formulate meaning of representation. We also hope the frame of representation articulated here may serve as a guide for designing new curricular activities and materials. There are many opportunities in our chemistry laboratory and classroom learning environments for making explicit reference to the process of creating representation as outlined in this paper. We also suggest that more research is needed in this area to develop the supports necessary to help students understand the reasoning processes and skill needed for connecting macroscopic and submicroscopic domains of knowledge.

AUTHOR INFORMATION

Corresponding Author

Mitchell R. M. Bruce − *Department of Chemistry and the RiSE Center, University of Maine, Orono, Maine 04469, United States;* orcid.org/0000-0002-6428-3842; Email: mbruce@maine.edu

Authors

Alice E. Bruce − *Department of Chemistry, University of Maine, Orono, Maine 04469, United States;* orcid.org/0000-0002-4556-8180

Joseph Walter − *the RiSE Center, University of Maine, Orono, Maine 04469, United States*

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.1c00292

Notes

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