Chapter 3
Exploring Mechanistic Reasoning in Chemistry

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Abstract Science educators across the world recognize the importance of developing students' ability to build arguments and explanations using scientific models. However, the type of mechanistic reasoning that we would like students to develop is challenging for many learners because it demands the simultaneous analysis of multiple factors operating at different scales. In this contribution, we summarize the major reasoning challenges that we have uncovered in our studies focused on the analysis of students' ability to use structure-property relationships to build mechanistic explanations about chemical substances and phenomena. Our investigations have revealed that students at all educational levels often rely on implicit knowledge and reasoning strategies to simplify tasks. In particular, they tend to apply quick heuristics that facilitate decision-making and intuitive schemas that simplify the construction of inferences. The three most common types of heuristics used by the participants in our studies include recognition, similarity, and one-reason decision-making. The most dominant intuitive schemas elicited by our research are an additive property schema and a centralized causality schema.

Introduction

Science education reform efforts in the past 20 years have stressed the need for students to actively engage in generating arguments and building explanations of relevant phenomena using scientific models (NRC 2007, 2011, 2013). Students' initial explanations of a process or event will likely include a variety of nonnormative ideas, some more productive than others. However, by asking students to express and discuss their ideas in public, teachers can assess student understanding, provide formative feedback, and better scaffold student learning (Windschitl et al. 2012). In this environment, a teacher's ability to notice more or less productive ways of thinking and to effectively respond to and build upon the ideas that students express strongly depends on her or his knowledge of how novice learners and

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experts in the field reason about the systems and processes under consideration (Coffey et al. 2011; Robertson et al. 2016).

Explanations of natural phenomena generated by scientists in different disciplines tend to be mechanistic in nature (Russ et al. 2008). These mechanistic accounts invoke the existence of specific agents (e.g., atoms, molecules, cells, organs) with particular properties (e.g., mass, charge, selective permeability) that determine how different agents interact with each other and the types of processes or activities in which they participate (Machamer et al. 2000). Mechanistic explanations are highly valued in science because they can be used to describe, explain, and predict the behavior of many systems of interest. Unfortunately, research in science education has shown that students often struggle to build mechanistic accounts of natural phenomena (Bolger et al. 2012; Grotzer 2003; Talanquer 2010) and that few science teachers know how to foster, scaffold, and assess students' development in this area (Robertson et al. 2016; Russ et al. 2009).

To better support the work of chemistry teachers and students when engaging in the construction of explanations, our research group has sought to characterize major roadblocks in the elaboration of mechanistic accounts of chemical phenomena. In particular, we have focused our attention on the characterization of patterns of reasoning that affect students' ability to explain and predict physical and chemical properties of substances using chemical models of the composition and structure of their submicroscopic components. The ability to build arguments and explanations based on structure-property relationships is a core competence in chemistry, and it is thus critical for teachers to recognize the types of difficulties that students face in developing and applying this type of reasoning. The central goal of this contribution is to summarize the reasoning challenges that we have uncovered and to discuss their implications for chemistry education at the secondary school and college levels.

Expert Reasoning About Structure-Property Relationships

Chemical scientists have developed a variety of models to explain and predict the physical and chemical properties of the different substances in our surroundings. Many of these models describe the composition and structure of matter at submicroscopic scales (Taber 2013a; Talanquer 2011). It is proposed, for example, that many pure chemical compounds are composed of myriads of identical particles (e.g., molecules, ions) in constant motion and interaction. The composition and structure of these particles are assumed to be unique for each type of substance and responsible for its macroscopic properties. A considerable amount of practical and theoretical efforts are thus invested in building composition-structure-property connections.

Chemical models of submicroscopic structure are mechanistic in nature. A specific set of agents, such as electrons, atoms, ions, and molecules, are defined and used to build mechanisms that explain how and why processes of interest (e.g., phase transitions, chemical reactions) happen. Relevant agents are assumed to have certain properties that determine their behaviors. Many of these properties are implicit rather than explicit, such as electrical charge, electronegativity, polarity, and polarizability. These properties affect how an agent interacts with other agents of the same or different types. These interactions, in turn, determine how a large collection of agents may respond to changes in their environment. For example, how their spatial and speed distributions may change when energy is exchanged with the surroundings.

Many models of chemical systems assume that the properties of a macroscopic sample of a material "emerge" from the random interactions and configurations that its submicroscopic components can adopt under particular conditions (Luisi 2002). This assumption implies that observed macroscopic properties differ from the properties attributed to the individual particles that compose the system. For example, the flexibility of a plastic is not explained as resulting from the flexibility of its individual molecular components but rather as emerging from the specific arrangement of and interactions between the myriads of molecules that make up the material. Nevertheless, the nature of these arrangements and interactions may often be inferred from the composition and structure of the individual particles.

Mechanistic explanations in chemistry frequently involve shifting between different scales of description of the agents, interactions, and processes that are invoked to explain or predict a phenomenon (Gilbert and Treagust 2009; Taber 2013a; Talanquer 2011). To illustrate this point, let us look at an explanation for why oil does not dissolve in water. As we begin our explanation, we may pay attention to the atomic composition and structure of a single molecule of each substance (analysis at a molecular scale). This information can be used to infer how electronic charge is distributed between the different atoms that comprise each molecule (analysis at an atomic scale) and thus make claims about molecular polarity and polarizability (analysis at the molecular scale). These inferred properties support predictions about the nature and relative strength of the intermolecular forces between different types of particles and allow us to evaluate whether the mixed or the unmixed states are more likely to be observed. However, the likelihood of mixing also depends on the extent to which the process increases or decreases the number of configurations that the collection of interacting particles can adopt (analysis at the multi-particle scale). In general, the construction of sound mechanistic explanations of chemical phenomena demands the analysis of interactions and processes occurring at the atomic, molecular, and multi-particle scales. We can surmise that such explanatory effort may be a daunting task for many learners, as well as a major instructional challenge for the teachers who seek to engage students in that type of reasoning.

Novice Reasoning About Structure-Property Relationships

Answers to questions involving structure-property relationships demand the identification of the various compositional and structural factors that are relevant in explaining or predicting the macroscopic properties of the substances of interest. In general, decisions need to be made about what factors to consider, and inferences should be built about the relative effects of these factors on the properties of interest. Our research studies have revealed that many students struggle with these types of multivariate problems in chemistry. Rather than applying explicit mechanistic reasoning based on scientific models, they often rely on implicit knowledge and reasoning strategies to simplify the tasks. In particular, they tend to apply quick heuristics that facilitate decision-making and intuitive schemas that simplify the construction of inferences. Major research findings in each of these two areas are summarized in the following paragraphs.

Heuristic Strategies

Research on human reasoning in social contexts has shown that people often rely on fast and frugal heuristics to make judgments and decisions (Kahneman 2011). These heuristics are tacit strategies for searching, selecting, and acting on relevant cues when making decisions. They can be thought of as implicit rules of thumb for quickly making choices under conditions of limited time, knowledge, or motivation to complete a task (Todd and Gigerenzer 2000). For example, we often rely on a "recognition" heuristic when buying a new product sold by different brands: we tend to choose the brand that we recognize despite the lack of information about the actual quality of all choices. The use of heuristic strategies often leads to reasonable decisions in diverse contexts, but it is also responsible for a variety of biases in judgment and decision-making. Although different heuristic strategies have been identified, they seem to share a similar cognitive mechanism (Morewedge and Kahneman 2010).

When asked to make a choice given limited time and information, the human mind tends to look for explicit and implicit differences between existing options, processing first those features that are more salient to an individual (Oppenheimer 2008). The most salient features are likely to include explicit characteristics, such as the relative size of objects, or familiar characteristics, such as the name of a known brand. During this search, our mind seeks to associate the noticed salient feature with the actual quality under evaluation. For example, in deciding whether Peter or John is more generous, our mind may first process the fact that Peter invited us for lunch 2 days ago. This action is likely to be associated with generosity in our mind, biasing our choice toward Peter. These cognitive processes unconsciously lead us to substitute a difficult question (e.g., who is more generous?) by a simpler one (e.g., who invited us to lunch recently?). In general, the choices that people make are strongly influenced by the features that are most salient to them in a given context and by the implicit associations made in their minds (Kahneman 2011).

We have been interested in exploring the extent to which chemistry students rely on heuristic reasoning rather than on mechanistic reasoning when engaged in making judgments, decisions, and predictions in chemical contexts (Talanquer 2014). Through questionnaires and individual interviews with college students who have completed general chemistry and organic chemistry courses at our university, we have investigated how they make decisions about the relative values of physical and chemical properties of different sets of substances. For example, how they decide which chemical compound in a set will have the highest melting point, be most soluble in water, or be the strongest acid (Maeyer and Talanquer 2010; McClary and Talanquer 2011). We have also analyzed how they decide which chemical reaction in a group will be most thermodynamically favored (Maeyer and Talanquer 2013). Making these choices demands the application of relevant structure-property relationships as well as properly weighing the effects of different variables. Our work has revealed that a large proportion of college students consistently rely on heuristic reasoning to make these types of chemical decisions, eluding the application of mechanistic reasoning.

The three most common types of heuristics used by the participants in our studies include recognition, similarity, and one-reason decision-making. When using *recognition*, students seem to apply the following rule when comparing and ranking chemical substances or processes: “If an option is recognized that exhibits the property under evaluation, place this option at the top or bottom of the ranking” (Goldstein and Gigerenzer 2002). For example, when comparing the acid strength of HCl, HBr, and HI, a significant number of general chemistry students selected HCl as the strongest acid simply because they recognized it as a strong acid of common use in the laboratory. Similarly, many students chose NaCl as the most soluble substance in a set also including NaBr and NaI based on their familiarity with the solubility of common salt. In our studies, “recognition” often provided a quick anchor for students to begin the ranking process reducing the likelihood of invoking structure-property relationships to justify decisions (Maeyer and Talanquer 2010).

Similarity is another heuristic often used by students to make and justify their choices. When applying this reasoning strategy, individuals identify similarities in explicit features of the substances or processes under analysis and use these similarities to guide their choices (Read and Grushka-Cockayne 2011). For example, in comparing the acid strength of HCl, HBr, and H_2S, students using this heuristic may judge HBr to be stronger than H_2S simply based on the similarity between the chemical formulas of the HBr and HCl (a substance that many students recognize as a strong acid). The use of similarity offers a shortcut for the more cognitive demanding task of identifying and weighing the effects of the different structural factors that affect acid strength (e.g., bond strength in the acid molecules, charge density and polarizability of the conjugate base molecules, etc.). Students who actually embark in this type of structural analysis frequently end up simplifying their reasoning by selecting a single variable on which to base their decision. Students who apply this *one-reason decision-making* heuristic (Gigerenzer and Gaissmaier 2011) search for a cue (one at a time) that can be used to differentiate between options (e.g., bromine is more electronegative than sulfur, H_2S has two hydrogen atoms) and then select the option with the highest or lowest cue value (e.g., HBr is a stronger acid than H_2S because the Br atom is more electronegative than the sulfur atom, H_2S is a stronger acid than HBr because it has more hydrogen atoms).

Heuristic reasoning is guided by the cues that individuals more easily identify when facing a problem. Thus, their reasoning may not be consistent across tasks as different types of features may be more salient in different contexts. What characteristics of the substances or processes represented in a chemistry task are most salient to students depend on their prior knowledge and experiences, which influence the assumptions they make about the nature and properties of the objects and events under consideration. Let us analyze some of the most common assumptions guiding novice chemistry students' reasoning.

Intuitive Schemas

Through constant interaction with the natural and social worlds, our mind develops implicit assumptions about the properties and behaviors of different entities and processes taking place in our surroundings (Chi 2008; diSessa 1993; Vosniadou et al. 2008). We assume, for example, that solid objects will always move in continuous trajectories and will not suddenly disappear into thin air (Spelke and Kinzler 2007). These types of assumptions guide the explanations and predictions we make when confronted with familiar and unfamiliar problems or situations. Imagine you were sitting in a chemistry class learning for the first time about the electrons and protons that make up an atom. In this situation, it is likely that your mind will tacitly categorize these subatomic entities as tiny solid particles and attribute to them the set of properties we associate with solid objects (e.g., moving coherently through space, persisting over time, being impenetrable). These implicit assumptions will help you make sense of what you are learning about entities you have never seen or interacted with before but may constrain your thinking when learning about, for example, the dual particle-wave nature of matter.

A significant part of our research has been focused on identifying and characterizing the implicit assumptions that novice chemistry students make when thinking about chemical systems and phenomena (Talanquer 2006, 2009, 2013a). Our findings suggest that some of these assumptions are tightly interrelated and can be conceived as intuitive schemas that guide but also constrain the explanations and predictions that students make (Talanquer 2015). Other authors in the conceptual change literature have identified these types of intuitive cognitive elements and discussed their critical role in the construction of knowledge. They have referred to them as framework presuppositions (Vosniadou et al. 2008), core hypotheses and ontological beliefs (Chi 2008), and core knowledge (Spelke and Kinzler 2007). These intuitive cognitive elements are frequently the source of alternative conceptions about specific systems or phenomena (Brown 2014; Chi et al. 2011; Coley and Tanner 2015; Taber and García-Franco 2010; Talanquer 2006), but they can serve as productive resources in the development of scientific understandings (Wiser and Smith 2016).

The intuitive schemas that seem to guide novice students' reasoning in chemistry often differ from the normative schemas used by experts to build structure-property relationships and seem to be resistant to change with training in the discipline. Results from our investigations indicate that the application of these schemas may depend on the nature of the question or problem faced by the students. Two of the most pervasive schemas elicited by our studies are the “additive property” schema and the “centralized causality” schema described below. These schemas have a strong influence on how students think about structure-property relationships.

Additive Property Schema This intuitive schema seems to guide students’ inferences about the properties of substances based on available information about their chemical composition and structure. The core interrelated assumptions that characterize this schema may be expressed as (Taber and Garcia-Franco 2010; Talanquer 2008, 2015):

(a) Chemical substances can be thought of as homogeneous aggregates or mixtures of diverse components (e.g., atoms, elements, ions, molecules, chemical bonds).
(b) Each component has inherent properties that are not affected by the presence of other components.
(c) The properties of each component are the same at all scales, from the macro to the submicroscopic scale.
(d) The properties of the substance result from the weighted average of the properties of all its components.

This “additive property” schema manifests in diverse ways when students engage in thinking about the relationship between chemical compositional and structural features and observable properties. For example, when college chemistry students were asked about the likely color, flavor, or smell of the product of a chemical reaction, the majority of them selected an answer consistent with the assumption of simple combination of properties of the reactants (e.g., the reaction between a blue reactant and a yellow reactant produces a green product) (Talanquer 2008). This response was common not only among novice college students but also among students who had completed 1 and 2 years of chemistry courses at our university (Talanquer 2013a). Similarly, these types of students inferred that a substance like silver chloride (AgCl) was likely to be shiny and malleable due to its silver content and that methanol (CH_4O) or ethanol (C_2H_6O) was more combustible than methane (CH_4) because their molecules contained oxygen, a substance they assumed to be flammable (Banks et al. 2015; Cullipher et al. 2015).

When learners apply an “additive property” schema, they think of the components of a chemical system as noninteractive parts with fixed properties. For example, they think of molecules as composite static objects that require energy to be assembled, and the larger the number of atoms in the molecule, the larger the amount of energy that needs to be invested to synthesize it (Maeyer and Talanquer 2013). When making judgments about the chemical reactivity of a molecular entity, students who apply this intuitive schema tend to pay attention to the number of atoms of a certain type which are seen as responsible for particular behaviors. For example, the more electronegative atoms are present in a molecule, the more reactive the molecule will be, or the more acidic protons a molecule has, the stronger acid it will be. The "additive property" schema supports reasoning based on a one-reason decision-making heuristic, where a single property of a component is used as cue to make inferences of the form "more A-more B" (Cooper et al. 2013; Stavy and Tirosh 2000).

The "additive property" schema applied by novice learners is substantially different from the "emergent property" schema held by expert chemists who think of atoms, molecules, and chemical substances as dynamic collection of interacting particles, with properties that emerge from such interactions. When using an emergent property schema to reason about a chemical system, inferences about properties are built based on the analysis of potential interaction between components rather than on the mere identification of the types of constituents and the quantification of their amounts. Research in chemistry education suggests that the shift from an "additive property" to an "emergent property" schema is not easy for many learners. We have found students at different educational levels expressing ideas that suggest they hold an additive property schema when reasoning about chemical substances and processes (Banks et al. 2015; Cullipher et al. 2015; Talanquer 2008). However, more advanced students tend to think of some properties in additive ways while thinking about other properties using an emergent property schema. For example, they may explain the difference in boiling points between CH_4 and CH_4O based on the relative strength of intermolecular interactions between molecules of these compounds, while attributing higher combustibility to CH_4O simply based on the presence of an extra oxygen atom in the molecules of this compound. These results suggest that the shift from one schema to the other is gradual and property dependent.

Centralized Causality Schema Students' reasoning about why and how physical and chemical processes happen based on compositional and structural cues is often guided by an intuitive schema based on the following interrelated implicit assumptions (Grotzer 2003; Resnick 1996; Talanquer 2006, 2013b):

(a) Processes are caused or driven by an active agent that can either orchestrate events or create conditions to enable them. This active agent acts on one or more passive agents.
(b) Processes are conceived as a linear chain of sequential events resulting from the action of one or more protagonists.
(c) The active agent tends to act purposefully, seeking to achieve some goal that will allow the system adopt a more desirable state.

This way of thinking has been elicited in different contexts, from asking students to make sense of bonding patterns in chemical compounds to asking them to explain why certain compounds react with one another. For example, chemistry students commonly think that ionic compounds are formed in a process in which some active atoms take away electrons from other more passive atoms that willingly donate their electrons. Such electron exchange is judged to occur because each type of atom "wants" to acquire a full valence electron shell (Taber 1998, 2013b; Talanquer 2013b). In our investigations of how students think about why and how different types of chemical reactions happen, the most common way of thinking expressed by undergraduate and graduate chemistry students rested on the assumption that substances react with each other in order to become more stable (Yan and Talanquer 2015). Highly reactive substances were often seen as the initiators of chemical processes that would take them to lower energy states. Within this schema, students consider that molecules of an acid donate a proton to molecules of a base in order to become more stable, and oxidizing agents take electrons from reducing agents for the same purpose. Stability is often associated with reduced energy, and thus a system's desire to reduce its energy is judged as the major driver for chemical change (Weinrich and Talanquer 2015).

As was the case with the "additive property" schema, the results of our investigations reveal that the application of a "centralized causality" schema is more common when thinking about some types of systems than others. For example, undergraduate and graduate chemistry students are more likely to apply this schema when thinking about reactions in which two substances combine to form a single product (combination reactions) than when analyzing processes in which two substances participate in a double displacement reaction. In this latter case, students are more likely to invoke a mechanism based on attraction and repulsion of charged particles to explain the process (Yan and Talanquer 2015). This result suggests that the intuitive "centralized causality" schema loses strength as explanatory tool on a case-by-case basis as students assimilate alternative mechanisms to explain chemical processes.

One can expect that students will struggle to develop more normative ideas about why and how physical and chemical processes happen using compositional and structural cues. Mechanistic explanations in chemistry typically involve the analyses of two of more processes occurring simultaneously across the system. Some of these processes may be conceptualized as opposite to each other (e.g., evaporation versus condensation, forward reaction versus backward reaction). The net outcome of these processes is determined by internal and external constraints that affect the relative probability of different random events. Observable patterns at the macroscopic level emerge from the continuous and dynamic random interaction of particles at the submicroscopic level. These interactions have equal status, with no recognizable "leaders" or "enablers." The required analyses are multivariate and multiscale in nature and thus demand high cognitive effort. Students' minds tend to simplify this task by focusing on a single agent and a single process, thinking at a single scale, and attributing preferentiality to probable outcomes.

Conclusions and Implications

The type of mechanistic reasoning that we would like our students to apply in chemistry classrooms is challenging for many learners because it demands the analysis of multiple variables and simultaneous processes. Additionally, it requires that students build connections between agents, properties, and processes defined at different scales (Taber 2013a; Talanquer 2011). These types of mechanistic explanations are quite different from the types of explanations we commonly build in our daily lives to make sense of the differences in properties and behaviors of the diverse entities and events happening in our surroundings. The human mind often develops implicit reasoning strategies to facilitate judgment and decision-making (Kahneman 2011), as well as tacit assumptions about the nature of things that guide the construction of inferences (Spelke and Kinzler 2007; Talmy 1988). These same heuristics and assumptions seem to guide students' thinking in the classroom and may constrain the application of more sophisticated mechanistic reasoning.

The results of our research suggest that novice learners tend to conceive chemical substances as composite objects and explain their properties and behaviors in terms of the inherent properties and behaviors of their individual components. This is not very different from how we make sense of the differences we observe in objects in our surroundings (Cimpian and Salomon 2014). We assume, for example, that the different colors in the wings of butterflies are due to the presence of different colored pigments, rather than considering that those colors actually emerge from interactions between wing materials and solar light. Our thinking about the changes that take place around us is also similar to that expressed by students when reasoning about physical and chemical changes in the classroom. We tend to think of larger, stronger, and faster objects as having more agency than smaller, weaker, and slower ones (Talmy 1988). We also tend to attribute intentionality to processes when there is none, like when we assume that plants turn toward the sun to get more light or that ants communicate with each other to gather their food (Kelemen and Rosset 2009). The assumptions that we make affect the features of a system or phenomenon to which we pay attention, biasing our judgments and decisions. Heuristic reasoning is as pervasive in our daily lives as it is in the classroom.

Our studies indicate that students develop the ability to use normative mechanistic reasoning to think about chemical systems and phenomena, but this ability seems to develop slowly and in pieces (Weinrich and Talanquer 2015; Yan and Talanquer 2015). This is, students learn to think in normative mechanistic ways about some specific processes while applying intuitive schemas to reason about others. This fragmentation may be due in part to our traditional approaches to teaching chemistry which focus more on acquisition of factual knowledge than on the development of productive ways of thinking in the discipline. Students tend to be confronted with mechanistic reasoning in isolated situations (e.g., explaining why a substance dissolves in water or why a chemical reaction reaches equilibrium), but there is no systematic effort to help them develop mechanistic frameworks that can be applied across different types of phenomena.

Traditional chemistry courses are organized as a sequence of topics (e.g., atomic structure, chemical bonding, chemical reactions) rather than around fundamental ways of reasoning in the domain. Teachers tend to emphasize the acquisition of descriptive knowledge and basic problem-solving skills. In these traditional environments, students learn to, for example, balance chemical equations, calculate amounts of substances, draw Lewis structures, and assign oxidation states. There are far fewer opportunities for students to engage in building arguments and explanations to make sense of properties and phenomena in relevant situations (Sevian and Talanquer 2014; Talanquer and Pollard 2010). Even when they do, few teachers are prepared to press students to generate mechanistic accounts, support learners in these efforts, and create activities that help them build generalizable ways of thinking that can be applied across different contexts (Russ et al. 2009; Robertson et al. 2016).

There is evidence to support the claim that students can engage in sophisticated mechanistic reasoning when given opportunities to do so in scaffolded learning environments. In these types of classrooms, students are confronted with authentic problems and asked to build explanations or design solutions using models (Windschitl et al. 2008, 2012). Teachers implement activities that elicit students' ideas and make their thinking public. Shared ideas can then be analyzed and challenged if necessary. Many students often express productive ways of reasoning that can be used to build more normative understandings (Wiser and Smith 2016). Comparing and contrasting different ways of explaining a system or phenomenon helps students identify the scope and limitations of different types of reasoning (Chi et al. 2011). Engaging students in collaborative construction of ideas has been shown to be highly successful in fostering the development of meaningful understandings (NRC 2005; Chi and Wylie 2014).

Changing the teaching approach, however, is only a part of what is needed to strengthen students' ability to engage in normative mechanistic reasoning. Chemistry educators and chemistry education researchers also need to more carefully reflect on the type of mechanistic reasoning that would be most productive for students to develop. There are major ways of explaining and inferring chemical properties and phenomena based on structure-property relationships that need to be made more explicit to both teachers and students (Talanquer 2015). Chemistry curricula could be modified to use these fundamental ways of thinking as central axes in the organization of the core ideas discussed and the major activities implemented in the classroom. A focus on fundamental mechanisms would help students better understand how some basic ideas in chemistry can be used to make sense of the properties of many diverse substances and a wide range of phenomena.

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