

Threshold Concepts in Chemistry: The Critical Role of Implicit Schemas

Vicente Talanquer*

Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721, United States

ABSTRACT: Threshold concepts are conceived as cognitive portals to new and previously inaccessible ways of thinking in a domain. They are transformative, integrative, irreversible, and troublesome concepts that open the door to highly productive ways of thinking in a discipline. Mastering threshold concepts in chemistry demands the construction of diverse cognitive elements, including implicit schemas that guide and constrain how students think about chemical substances and processes. The central goal of this paper is to highlight five critical shifts in students' implicit schemas that should be fostered to support mastery of major threshold concepts in chemistry.



KEYWORDS: General Public, Chemical Education Research, Misconceptions/Discrepant Events, Learning Theories

■ INTRODUCTION

In recent years, the idea of “threshold concepts” has gained prominence in discussions about learning, teaching, curriculum, and assessment in several disciplines, from economics to engineering to biology.^{1–3} The core assertion is that there are certain concepts within each discipline that resemble portals to new and previously inaccessible ways of thinking that are central to the domain.^{4,5} As a result of crossing the portal, learners acquire a new way of looking at the world and generating meaning. In general, the comprehension of a threshold concept is expected to involve a major transformation in the manner in which someone understands or interprets relevant systems and phenomena in a discipline. Identifying and characterizing threshold concepts are then seen as critical steps in curriculum design. Examples of threshold concepts in different domains include “Cellularity” in Biology,⁶ “Steady State” in Biochemistry,⁷ “Format as Process” in Information Literacy,⁸ and “Opportunity Cost” in Economics.⁹

Threshold concepts are assumed to have the following characteristics:^{1–9}

- Transformative—Their understanding causes a significant shift in perspective and ways of thinking about a subject.
- Integrative—Their understanding brings together various concepts and ideas.
- Irreversible—Once understood, the concepts become central to the ways of thinking of an individual and are unlikely to be forgotten.
- Troublesome—Many threshold concepts seem counter-intuitive and are difficult to understand.
- Bounded—Many threshold concepts are specific to a discipline.

Some of these features are similar to those suggested as filters for selecting big ideas or enduring understandings in curriculum

design.¹⁰ In particular, big ideas are often expected to (i) be at the heart of a discipline, (ii) have wide-ranging explanatory power, and (iii) be difficult to grasp. Given the similarities in defining criteria, one must question whether “threshold concept” and “big idea” are just different labels for the same curricular construct. From my perspective, the overlap between these two concepts is substantial, but each of them directs our attention to different aspects of the subject matter.

The reference to “big ideas” tends to highlight the importance of focusing instruction on the development of understandings that have considerable explanatory power, provide the basis for prediction and decision-making in a wide range of relevant contexts, and are intellectually satisfying because they generate the answers to many questions of personal or social interest. Big ideas focus our attention on desirable learning targets and outcomes. On the other hand, the idea of “threshold concept” emphasizes the importance of embarking students on journeys that transform their ways of thinking in highly productive manners within a domain. Threshold concepts not only identify desirable learning targets but also draw our attention to those concepts and ideas whose comprehension will likely involve profound conceptual change.^{9,11} The characterization of a threshold concept thus demands more than the mere description of the new ways of thinking and practice that such concept will enable. It also requires outlining the critical cognitive elements that need to be constructed and integrated by an individual to successfully develop the type of thinking that the threshold concept enables.¹² In this paper, I use the term “conceptual threshold” to refer to the cognitive elements and processes that support the construction of a threshold concept and use the metaphor of “crossing a conceptual threshold” to signify the acquisition or development of such elements.

If we were to ask chemistry teachers and instructors to list some threshold concepts in chemistry, it is likely that many of them would include concepts such as “Atomicity”, “Chemical Bonding”, “Intermolecular Forces”, and “Chemical Equilibrium”. The meaningful understanding of these concepts can radically change the way in which someone thinks about chemical substances and reactions. These same concepts also encapsulate big ideas in chemistry as described in past^{13,14} and recent^{15–17} education standards and content maps.^{18,19} However, thinking of these concepts as threshold concepts invites us to carefully analyze what is needed to, metaphorically speaking, help students cross a conceptual threshold. In this contribution, I focus my attention on the description of a specific set of cognitive elements that educational research suggests are critical for developing core threshold concepts in chemistry but are not typically described in common educational resources, such as education standards and chemistry textbooks. I have labeled these elements “cross-cutting threshold schemas”. They are “crosscutting” because they are relevant for the understanding of ideas in several areas, they are “threshold” because they are doors to new ways of thinking about entities and processes, and they are “schemas” because they encompass a web of interrelated implicit assumptions that guide but also constrain how people think about systems and phenomena.

■ CROSSING A CONCEPTUAL THRESHOLD

Chemistry teachers and instructors often express their disappointment with their students’ learning in rather general ways. They might say, for example, “My students do not understand chemical equilibrium”. Despite the vagueness of this statement, other chemistry instructors are likely to understand what their colleague means. Tacitly, this statement is letting us know that the students are unable to express and apply the rich and productive thinking that the concept of “chemical equilibrium” enables. The students have not yet crossed the conceptual threshold that leads to the meaningful understanding of such concept. However, it is likely that many of them have developed some understandings that are needed to complete the journey. They may know, for example, what an equilibrium constant is and how it can be calculated. They may recognize the existence of forward and backward chemical processes in a chemical system. Many students may be on their path to the desired destination, but they are stuck on different points along the way.

Moving through a conceptual threshold is challenging because learners will likely have to dismantle, set aside, coalesce, or separate existing assumptions, concepts, and ideas while building new ones.^{4,5,9} They have to not only construct the path to the threshold concept but also select the proper elements to build it and learn how to put them together. Learners do not just cross a conceptual threshold; they build it as they move through it without a clear sense of where and when the exit will appear. Understanding “chemical equilibrium” is not about collecting the right pieces of knowledge and putting them together using a simple and straightforward instruction manual handed to them by an instructor. Mastering a threshold concept demands considerable investment of effort and learning should be carefully scaffolded to facilitate the construction and assembly of such concept.

A threshold concept is a complex cognitive construct that can be expected to involve a variety of (i) conceptual, (ii) epistemological, and (iii) ontological elements.²⁰ The nature

of these different types of cognitive elements has been described and discussed by a variety of authors interested in conceptual change.^{11,21–23} These elements support productive reasoning in a given domain, but they may also lead people to build flawed mental models or to hold alternative conceptions about relevant entities and phenomena. Although different researchers may disagree on the level of integration of these different elements in students’ minds, from highly integrated in the form of framework theories²¹ to somewhat organized around ontological categories²² to highly fragmented as knowledge-in-pieces,²³ most authors agree on the existence of different types of cognitive resources that guide but also constrain reasoning. Some of these cognitive constructs are explicit and, thus, available to conscious thought. Others are implicit and influence reasoning without an individual’s awareness.²⁴ Mastering a threshold concept likely demands the development, reorganization, or reformulation of many of these cognitive elements and, thus, may require radical conceptual change.^{11,22}

Conceptual Elements

Building and moving through a conceptual threshold requires the construction of basic concepts and ideas that pave the way to understanding. These types of conceptual elements are commonly listed in education standards^{13–17} and content maps,^{18,19} documents that summarize big ideas and enduring understandings in a discipline. Consider, for example, the threshold concept of “Atomicity” whose comprehension is critical for making sense, predicting, and controlling the properties of matter. Basic concepts and ideas associated with this threshold concept may include:^{18,19}

- “Matter consists of atoms that have internal structures that dictate their chemical and physical behavior.”
- “Atoms have unique chemical identities based on the number of protons in the nucleus.”
- “Atoms display a periodicity in their structure and observable properties that depend on that structure.”

These statements indicate that understanding “Atomicity” demands the construction and comprehension of concepts such as “atomic structure”, “periodicity”, and “chemical properties”. The development of these conceptual elements tends to be the focus of most teaching efforts in traditional chemistry classrooms and of chemistry education researchers interested in exploring and assessing student learning and understanding.^{25–28}

Epistemological Elements

Recent education standards and content maps also make explicit, although frequently in very general terms, the types of disciplinary practices that learners have to master to comprehend how knowledge is established and how explanations and arguments are built in a discipline (epistemological elements).^{16–19} For example, to meaningfully understand “Atomicity” students need to differentiate between models and reality, comprehend how experimental information about light-matter interactions can be used to build arguments and theoretical models of atomic structure, and understand that these models may change based on new experimental information. These epistemological elements are critical in shaping and promoting the passage through the conceptual threshold.^{9,12,20,29}

Ontological Elements

The mastery of a threshold concept also depends on the use of proper schemas to think about the nature of the entities and processes in the systems under consideration, and of the relationships between such components (ontological elements).²² For example, do learners conceptualize electrons in an atom as solid objects or as standing waves? Do they conceive electron energy as a continuous or as a quantized property? Do they think of the strength of interactions between protons and electrons in an atom as fixed or as variable quantities? The assumptions that people make about the nature of things have a major impact on how they interpret a concept or idea.^{22,24,30} The statement “matter consists of atoms that have internal structures that dictate their chemical and physical behavior” might mean very different things to individuals who conceptualize atoms as solid objects with rigid internal structures than to people who think of atoms as dynamic interacting systems.

Research in science¹¹ and chemistry^{24,30–33} education suggest that many of the challenges that students face in crossing a conceptual threshold result from the application of implicit (i.e., tacit or unconscious) schemas that differ from those on which the targeted understandings actually rest. The problem is exacerbated by the lack of explicit description, analysis, and discussion of such sets of implicit assumptions in traditional curricular and teaching approaches; these types of threshold schemas are not overt components of education standards, content maps, or topic lists. Somehow, it is expected that the right schemas will naturally develop or become clear when learners engage with the content. Unfortunately, that does not seem to be the outcome for a majority of students who often are found applying sophisticated disciplinary concepts (e.g., electronegativity, resonance, chemical energy) guided by rather intuitive schemas.^{25–28} Thus, it is the central aim of this paper to call attention upon this set of implicit cognitive elements and highlight some of the most critical schema shifts that need to be fostered in chemistry education.

The identification of the major schema shifts described in the next section was based on the analysis of existing research in chemistry education, particularly of review studies that summarized insights into students' implicit assumptions about the nature of submicroscopic entities and processes.^{20,25–33} Threshold concepts in chemistry (e.g., chemical bonding, chemical equilibrium) often provide mechanisms for connecting structures and processes at the submicroscopic level with the properties and behaviors of substances at the macroscopic level. Thus, the analysis focused on those studies that elicited students' implicit ways of reasoning about structure–property relationships.

CROSSCUTTING THRESHOLD SCHEMAS

Modern chemistry relies on submicroscopic models of matter to describe, predict, explain, and control the properties and behaviors of chemical substances. These models assume that substances are comprised of myriads of particles in constant movement and interaction with each other. The meaningful comprehension of these models of matter and its transformations is at the core of many of the conceptual difficulties that students have in understanding chemistry.^{25–28} The connection between the properties of a macroscopic sample of a material and the properties of the submicroscopic particles that constitute it is not straightforward. Moving between the macroscopic and submicroscopic levels of description in

chemistry is rather challenging.^{34,35} It demands radical shifts in the way people intuitively think of matter and its changes.³⁶ Consequently, the crosscutting threshold schemas described in this section mostly refer to changes in the ways in which learners need to conceptualize both the submicroscopic world and the representations that chemist use to depict it. These schemas are often implicit (i.e., students unconsciously apply them) and likely act in conjunction in many situations.

Several of the threshold schemas that are described in the following paragraphs are needed to understand the properties and behavior of complex systems comprised of multiple and diverse components in dynamic interaction. Thus, they are crosscutting schemas that not only support the mastery of different threshold concepts in chemistry but are also critical for the understanding of fundamental concepts and ideas in other areas such as Biochemistry^{7,37} and Biology.⁶ From this perspective, they may be ideal educational targets to better support learning across multiple disciplines. To more clearly characterize the cognitive shifts that need to be facilitated in chemistry education, the presentation that follows includes a description of the schemas that commonly sustain reasoning in opposite sides of the highlighted thresholds.

From an “Additive Property” to an “Emergent Property” Schema

Research in chemistry education suggests that novice learners tend to think of chemical substances as homogeneous aggregates or mixtures of diverse components (e.g., atoms, elements, molecules, chemical bonds) with specific properties. The properties of a substance are then often assumed to result from the weighted average of the properties of its components.^{30,38} Using this schema, a chemical compound that is the product of the reaction between a blue and a yellow substance will be expected to be green,³⁸ and a substance like silver chloride (AgCl) may be predicted to be shiny and malleable due to its silver content.³¹ Properties of a material are judged to be the same at all scales and changes in the properties at the macro level are thought to be similar to changes in the properties at the submicroscopic level: if a solid expands, its constituting particles also expand; if a substance changes color, its atoms or molecules do the same.^{25–28} This “additive property” schema manifests in various ways in different contexts. For example, it is common for chemistry students to think that the greater the number of atoms in a molecule the more energy is needed to synthesize it.³⁹ Similarly, many students consider that the more chemical bonds a molecule has, with these bonds seen as the components that contain chemical energy, the more energy the molecule will release when its bonds are broken.

When learners apply an “additive property” schema, they think of the components of a system as noninteractive parts with fixed properties; they treat the system as a composite static object. This schema is substantially different from that held by expert chemists who think of chemical systems (e.g., atoms, molecules, actual substances) as dynamic collections of interacting particles, with properties that emerge from such interactions.⁴⁰ Under this “emergent property” schema, the properties of a system are not easily predictable because they are sensitive to the number, type, and distribution over space and time of interacting components. Inferences about properties are based on the analysis of the likely outcome of interactions between constituents rather than on the mere identification of their types and amounts. To a large extent, the

system under analysis is conceived as a dynamic process rather than as a static object, and measurable properties represent average values of targeted quantities (e.g., number of particles per unit volume, kinetic energy per particle) over the many configurations that system particles adopt in a measurement's time span.

The shift from an "additive property" to an "emergent property" schema does not seem to be easy for many chemistry learners. A substantial number of college students commonly express ideas that suggest they still hold an additive property schema.^{30,38,39} Interestingly, students may think of some properties in additive ways (e.g., color, flammability) while applying an emergent property schema when thinking about other characteristics (e.g., density). Developing a sense of the actual mechanism that leads to the emergence of a given property seems to be important in enabling the shift from one schema to the other.^{41,42}

From a "Centralized Causal Process" to an "Emergent Process" Schema

While an "additive property" schema tends to dominate novice learners' reasoning about the properties of materials, a "centralized causal process" schema often guides students' thinking about the transformations of matter.⁴³ Within this schema, processes are viewed as driven by active agents that can either orchestrate events or create conditions to enable them.^{44,45} These agents are frequently conceived as having goals that should be met to reach a more desirable state.^{46,47} For example, students may think that an acid donates a proton to a base in order to become more stable, or that an oxygen atom always gains two electrons when reacting with other atoms so that it can have a full valence electron shell.⁴⁸ Highly reactive substances are commonly seen as the initiators in chemical reactions, and changes in the properties of a solution are often attributed to the active action of solute particles on solvent particles.⁴³

This centralized mindset about events and processes seems to be embedded in the manner in which humans think and talk about causation in everyday life.⁴⁹ We tend to describe changes as linear chains of sequential events resulting from the action of one or more protagonists who overcome challenges to meet their goals. This schema is quite different from the "emergent process" schema that has to be applied to understand physical (e.g., diffusion, boiling) and chemical (e.g., chemical equilibrium, molecular binding) processes in multiparticle systems.^{41,42} In these cases, observable patterns at the macroscopic level emerge from the continuous and dynamic random interaction of particles at the submicroscopic level. All of the interactions have equal status, with no recognizable "leaders" or "enablers", and various processes may occur simultaneously across the system. The outcome of these processes is determined by internal and external constraints that affect the relative probability of different random events.

Although there are instances of emergent phenomena involving collections of macroscopic objects (e.g., traffic jam, rumor spreading),⁵⁰ it is unlikely that people will easily recognize and transfer this process schema to think about changes in matter at the submicroscopic level. Regardless of the nature of a system's components, we can expect individuals to struggle to reconcile the existence of different behaviors at different levels of description (from cars moving forward while the actual traffic jams propagates backward to molecules reacting with each other while their average concentrations

remain constant). Many of these difficulties seem to stem from the inability to conceptualize how random changes at the component level may result in stable patterns of behavior at the system level. Explicit training on how to think about emergent phenomena may be needed to help students recognize when and how to apply the proper process schema.⁴²

From a "Homogeneous Population" to a "Varied Population" Schema

Novice learners tend to conceptualize the submicroscopic world as rather homogeneous and invariable.^{26,36,51} Molecules of a substance are conceived as identical rigid objects moving at similar speeds. Whenever a physical or chemical process occurs, molecules are likely thought of as undergoing the same change at the same time. When building explanations or making predictions, students' attention often focuses on the changes suffered by single representative molecules, making it difficult for learners to understand how several processes may be taking place simultaneously in a given system. This "homogeneous population" schema also hinders students' understanding of the critical effect that local temporary changes in individual molecules (e.g., induced dipole moments) or groups of molecules (e.g., density or energy fluctuations) have on the properties and behavior of matter.

The shift to a "varied population" schema demands that individuals recognize not only variability in the properties of individual particles in a system, but also the central role that this variability plays in making sense of a system's behavior. For example, understanding phase change and reaction kinetics hinges on the recognition of variability in the kinetic energy of particles, whereas analysis of spectroscopic data relies on the consideration of a variety of atomic and molecular distributions (e.g., isotopic composition, molecular orientation). To cross this conceptual threshold, students must comprehend how variability at different scales is a major source of change in multiparticle systems⁵² and understand how transformations that evolve in well-defined directions can actually emerge from random fluctuations in the spatial and energetic distribution of particles in a system.

From a "Intrinsic Chemical Property" to a "Extrinsic Chemical Property" Schema

It is common for novice learners to treat the chemical properties of a substance, or of its components (e.g., atoms, molecules), as intrinsic characteristics that determine their behavior under all conditions.^{25–28} For example, a strong acid is expected to be strong in all types of solutions; the molecules of a given chemical compound are assumed to contain a fixed amount of energy that is characteristic of every substance; a base may never behave like an acid. Chemical properties of substances are treated as absolute quantities that remain invariable from system to system in which such substances are present. In this "intrinsic chemical property" schema, the different environments in which chemical processes take place act as inert backgrounds upon which chemical reactions unfold.

The manner in which many students conceptualize chemical properties is quite different from the "extrinsic property schema" that guides expert reasoning in chemistry. The chemical properties of substances are, for the most part, extrinsic properties that depend on the nature of the environment in which substances are placed. They are relative properties that vary depending on the nature of the interacting species in a chemical system. Understanding how to think about such properties is difficult as it demands not only

recognizing their extrinsic nature but also making sense of the reference systems chosen to assign relative values. The arbitrariness with which these reference systems can be selected further adds to the confusion over the actual meaning of different reactivity scales and over the scope of their application (e.g., whether HCl should be thought as a strong acid in nonaqueous solutions). Little educational research has been completed in this area and it is needed to better support students moving through this conceptual threshold.

From a "Variation" to a "Conservation" Schema

People tend to be good at detecting changes in their environment and using those cues to build causal explanations.^{51,53} If something falls out of place, they look for an object or event that may have induced the movement; if their stomach hurts, they think about what they ate that may be responsible for their discomfort.²⁰ They seek explanations for the changes that they perceive, cueing on what is different before and after an event to identify potential causes and often disregarding what was conserved or remained constant during the process. People do not feel an urge to explain what they perceive as the natural state of things in their surroundings, but they spontaneously look for explanations to changes in the natural state of affairs.

A central goal of chemistry is to explain, predict, and control changes in the material world. Interestingly, the theoretical schemas that chemists have devised to accomplish such tasks often rely on identifying what is conserved during a process, rather than dwelling on what has changed. They apply conservation principles (e.g., mass, energy, electrical charge) to find relationships between a system's components before and after a process. They recognize and exploit the constancy over time and space of properties of a reacting mixture (e.g., equilibrium constants, chemical potentials) to build predictive models. Shifting from a "Variation" schema to a "Conservation" schema is not easy because it requires not only acknowledging the existence of conservation and constancy principles but also focusing the attention on implicit rather than explicit properties of chemical systems. Research in science⁵¹ and chemistry education^{25–28} has shown that student reasoning is highly constrained by explicit cues (e.g., changes in physical appearance) and that meaningfully understanding the conservation of implicit quantities is often rather challenging.

■ FINAL COMMENTS

The suggestion that there are threshold concepts in each academic discipline that open the door to productive ways of thinking in a domain invites us to identify these concepts and to characterize what is needed to master them. Such mastery will certainly demand the meaningful understanding of core conceptual elements, such as the idea of "intermolecular forces" if we want students to make sense of many properties of matter, or the concept of "chemical equilibrium" if they are to explain, predict, and control chemical processes in aqueous environments. There are other cognitive elements, however, that are equally critical in ensuring passage through conceptual thresholds in chemistry but are often overlooked. In particular, the central goal of this paper has been to highlight the importance of implicit ontological elements, depicted as crosscutting threshold schemas that shape the manner in which students conceptualize chemical substances and processes.

Recognizing the types of implicit schemas described and illustrated in this paper allows us to enrich and better focus the learning objectives for our courses, the instructional strategies that we consider, and our assessments of student understanding. It can also help in building integrated understandings across disciplines. Consider, for example, the recent work on threshold concepts in Biochemistry by Loertscher and collaborators.⁷ The understanding of the five threshold concepts that these authors identify (steady state, biochemical pathway dynamic and regulation, the physical basis of interactions, thermodynamics of macromolecular structure formation, free energy) is highly dependent on the development of the five expert schemas discussed in this contribution.

Discussions of what students should know or be able to do after completing our chemistry courses often remain at the conceptual level, without much reflection about the extent to which the ways of thinking we want students to develop are at odds with the implicit assumptions that they often make about how things work. Research findings in science and chemistry education suggest that this implicit knowledge plays a central role in the learning process as it shapes the construction of new understandings.²⁴ The five crosscutting threshold schemas described in this paper illustrate the distance that frequently exists between the implicit ways of thinking of novices versus experts in chemistry and the challenges that teachers and instructors face in helping students transform the ways in which they conceptualize the chemical world.

Helping students substantially move through the thresholds described in this paper demands major changes in what we teach and how we teach it, as well as in the strategies that we use to assess understanding. Current chemistry education at the secondary and college levels tends to follow a toolbox approach in which the major goal is for students to develop a set of rather isolated skills that are thought to be fundamental in chemistry, such as balancing chemical equations, solving stoichiometry problems, building electron configurations, drawing Lewis structures, and setting up ICE tables.⁵⁴ The core goals, essential questions, implicit assumptions, and ways of thinking of the modern chemical enterprise are buried deep below the traditional chores of school chemistry.⁵⁵

One of the main arguments for keeping the current state of affairs in chemistry education is that the basic skills traditionally taught are critical for later engagement in higher level thinking in the discipline. Many instructors also think that most of their students could not handle what they perceive as more challenging content. We should overcome the false dichotomy between the focus on basic skills and the focus on more authentic and relevant chemical thinking. For the past seven years, we have worked on the development and implementation of a general chemistry curriculum that seeks to engage students in the types of analysis and reflection that we think are needed to successfully cross critical conceptual thresholds.⁵⁶ Students who have completed these reformed courses have significantly outperformed their peers enrolled in traditional courses, in terms of both basic skills (as measured by ACS standardized exams) and conceptual understanding (as measured by research-based conceptual inventories).

If we want students to develop the powerful ways of thinking and problem solving in our discipline, we have to invest time unpacking students' views of the world and contrasting them with the fundamental schemas that sustain modern chemistry theories and practices.⁴² We need to transform our curricula to reduce the overemphasis on the accumulation of knowledge

and the development of isolated skills and open opportunities for students to build the conceptual, epistemological, and ontological elements that are needed to successfully master threshold concepts in our field. Engaging students in learning activities that demand that they analyze data, create models to make sense of the data, construct mechanistic explanations using such models, and build evidence-based arguments can help students question their implicit schemas and develop more sophisticated understandings.^{57,58} We should also revamp our assessment practices to challenge ourselves and our students to generate evidence of meaningful understanding. We need to uncover the essence of the content we teach, find ways to actively engage students in the discussion, analysis, and reflection of the fundamental assumptions guiding modern chemical thinking, and develop assessment instruments that better reveal where students stand within the conceptual thresholds we want them to cross.

AUTHOR INFORMATION

Corresponding Author

*E-mail: vicente@u.arizona.edu.

Notes

The authors declare no competing financial interest.

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