

Development and Assessment of a Molecular Structure and Properties Learning Progression

Melanie M. Cooper,^{*,†} Sonia M. Underwood,[†] Caleb Z. Hilley,[†] and Michael W. Klymkowsky[‡]

[†]Department of Chemistry, Clemson University, Clemson, South Carolina 29634-0973, United States

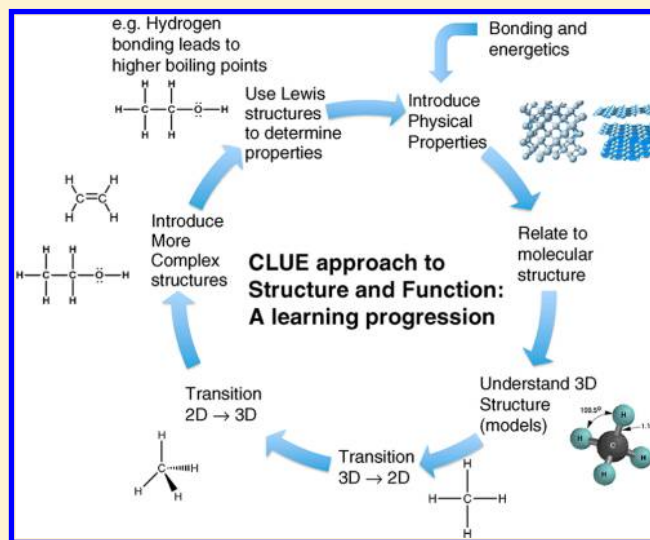
[‡]Department of Molecular, Cellular, and Developmental Biology, and CU Teach, University of Colorado, Boulder, Boulder, Colorado 80309-0347, United States

S Supporting Information

ABSTRACT: Previously, we found that: (i) many students were unable to construct representations of simple molecular structures; (ii) a majority of students fail to make the important connection between these representations and macroscopic properties of the material; and (iii) they were unable to decode the information contained in such representations. Assuming that lack of an understanding of the purpose of such representations inhibited students' meaningful learning, we have worked to address this "representation problem" explicitly in the context of a novel introductory general chemistry curriculum: Chemistry, Life, the Universe, and Everything (CLUE). CLUE includes a learning progression to help students master the relationships between molecular structure and bulk properties. Two methods were used to assess student learning: OrganicPad, a tablet-PC program that can recognize, record, and grade student free-form naturalistic structure drawings; and the Implicit Information from Lewis Structures Instrument (IILSI), a validated survey that asks students to identify the kinds of information they believe can be deduced from Lewis structures. A comparison of two statistically equivalent cohorts of students revealed that CLUE students show marked improvements (effect size, $r = 0.6$), over control students in their ability to construct structures. CLUE students were also significantly better at decoding the information that these structures contain. We present evidence that the improvements observed are due to the design and implementation of the specific learning progression rather than instructor effects.

KEYWORDS: High School/Introductory Chemistry, First-Year Undergraduate/General, Second-Year Undergraduate, Chemical Education Research, Learning Theories, Lewis Structures, Covalent Bonding, Molecular Properties/Structure

FEATURE: Chemical Education Research



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INTRODUCTION

The idea that a substance's molecular structure determines its macroscopic properties is a central premise of a wide range of molecular sciences. Nevertheless, students at all levels find it difficult to connect the visible, measurable properties of even the simplest compounds to various representations of their molecular-level structure.^{1,2} Even when students can demonstrate an understanding of a particular molecular system, most do not or cannot transfer their understanding to a new system.^{3,4} Students often rely on heuristics or surface level cues⁵ to answer questions rather than building their answer on a clear understanding of how molecular-level features can be used to predict macroscopic physical and chemical properties. While this problem may first appear in chemistry courses, the implications transcend chemistry; molecular macroscopic

structure–function relationships are key throughout the materials sciences, from engineering to drug design. As an example, most biology courses, beginning at the high school level, present representations of complex molecular structures, the implication being that students understand how to decode the information implicit within them. There is little evidence, however, that this is the case. We believe that, in part, student difficulties in interpreting representations of molecular structures stem from the traditional chemistry curricula in which this extremely complex construct is taught and assessed.

The path that students must take from a molecular formula to a prediction of properties involves at least eight distinct steps, each of which must be connected to the last, and many of

which require the application of sets of rules that may not have meaning for the students.⁶ An experienced chemist can look at a pair of molecular formulas, such as CH_3OCH_3 and $\text{CH}_3\text{CH}_2\text{OH}$, and deduce a wide range of properties and reactivities from them. Beginning students, however, must explicitly connect a long sequence of inferences in order to produce such predictions. This process may be particularly difficult for students who have come to believe that understanding chemistry (or for that matter, biology or biochemistry or physics) means memorization and pattern recognition. Therefore, the student must, perforce, rely on surface-level features, and use heuristics (rather than conceptual understanding) to make their predictions.^{5,7–9} It is our contention that students who cannot traverse the long road from molecular-level structure to property prediction are sentenced to a superficial understanding of chemistry and chemistry-dependent systems. It is likely they will not be able to transfer their current understanding to new situations. We suggest that this widely documented problem results in large measure from the fact that conventional teaching of structure–function relationships is fundamentally flawed: it does not take into account our understanding of how people learn, while dramatically underestimating the inherent difficulty in mastering quite abstract concepts.

Design of the Learning Progression

A growing acknowledgment among educators recognizes that difficult topics such as structure property relationships take time to master, and therefore need to be presented, worked with, and mastered in a learnable order. This approach, known as a learning progression,^{10–14} is an evidence–based description of pathways that are likely to lead to improved mastery of core ideas in science. Here, we present a description of the development and assessment of a learning progression based on our own findings and existing research, targeted at the connection between molecular structure, its representations (in particular, Lewis structures), and the ability to predict chemical and macroscopic properties. An important point is that we are not concerned about how the material is taught (for example, we accept that student-centered, active environments are generally more effective than passive lectures and computer generated multiple choice questions),^{15–18} but rather with *what* is taught, the order in which it is learned, what is emphasized, and the depth of understanding required to show that students have learned.

The Chemistry, Life, the Universe, and Everything (CLUE) curriculum is designed to develop a deeper understanding of a small number of core concepts. Likely numerous possible strategies involving specific sequences of materials exist, all of which could result in a coherent understanding of a particular difficult concept. More to the point, structure–property relationships involve an interconnected network of concepts that are all required for robust understanding (as demonstrated by the ability to effectively engage new scenarios, i.e., transfer). The sequence we have chosen for the CLUE curriculum begins with an introduction to bonding and the energy changes that accompany atomic interactions, that is, what happens when two atoms approach each other. One common misconception that students hold is that atoms form bonds because they “want” an octet, rather than because bonded atoms are more stable than unbonded ones. Students confuse the rules for the construction of Lewis structures with the reasons why bonds form (the decrease in system energy).⁹ This critical connection between

energy changes and atomic interactions is a core concept in the curriculum and reiterated whenever relevant (which is frequently).

Next, students are then introduced to properties of materials, such as diamond and graphite. How can substances formed from the same atoms display such different properties? The different models of bonding are then introduced, and used to explain how the molecular-level structure determines macroscopic properties. *Before* students learn to draw Lewis structures, they are introduced to the three-dimensional structures of simple molecules (such as hydrocarbons), by the use of models, both physical and computer-based. For example, they learn what tetrahedral geometry looks and feels like as they examine and draw representations of compounds such as methane and water from physical models, and compare these to computer-generated models of different types. It is only now that Lewis structures are introduced for what they are, namely, two-dimensional “cartoons” of the three-dimensional structures. We stress the fact that Lewis structures are merely a convenient way to represent something more complex. Students are asked to identify the implicit information contained in the structures. Once students are familiar with the translation from three-dimensional to two-dimensional representations, and the reverse process, more complex structures are introduced. As our prior studies have shown that students have trouble with even simple Lewis structure drawing,¹ we have confined the CLUE curriculum materials to structures with up to four bonds around an atom, and do not emphasize “extended octet” compounds. While structures such as the interhalogen ions or the noble gas compounds are interesting and important for chemists, we believe they are distractions for beginners and add to the complexity of the tasks, particularly because (in traditionally sequenced courses) they are often taught as “exceptions” to the “rules”.

When students are able to draw simple structures from a given molecular formula, they are introduced to the task of decoding the information that the formula contains. While some of this material is introduced in a way similar to that used by traditional courses (e.g., VSEPR to predict molecular shapes), an emphasis is placed on the sequence of actions required to extract the information implicit in the structure. That is, from a consideration of molecular shape and electronegativity of the component atoms, molecular polarity and intermolecular forces can be deduced. These connections are made explicitly in the CLUE curriculum, and are returned to throughout the two-semester course sequence. For example, in the second semester, while the traditional topics of kinetics, equilibria, and thermodynamics are “covered”, these topics are introduced in context with each other (not in separate chapters), and emphasis and examples are always linked back to the “big idea” of structure and function relationships. A full description of the CLUE curriculum materials can be found online.¹⁹

To assess the efficacy of this approach, we focused on two areas:

1. A comparison between a control and treatment cohort of student’s ability to draw Lewis structures.
2. A comparison between a control and treatment cohort of student’s student ability to use Lewis structures to predict properties.

A representation of the approach is shown in Figure 1.

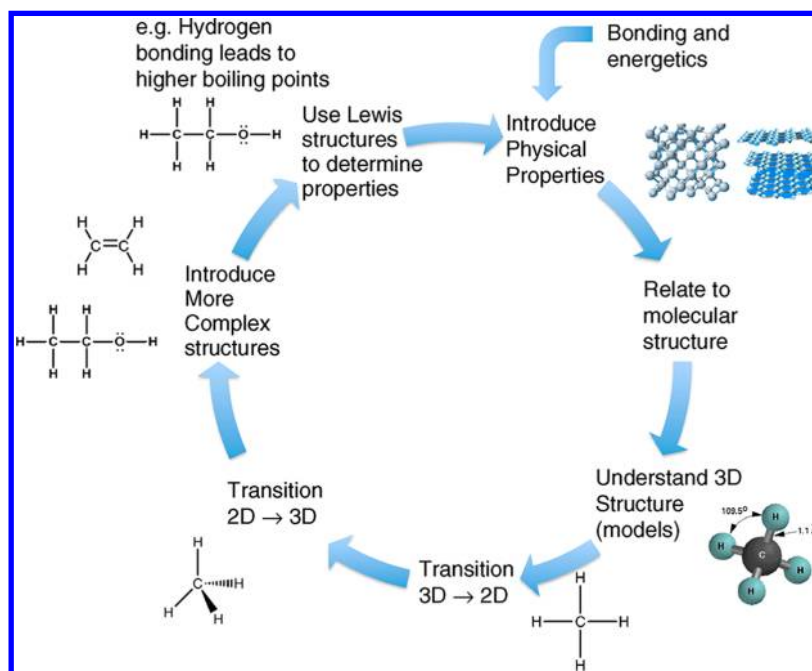


Figure 1. The CLUE learning progression for structure and function. Bonding is introduced first to emphasize that the reason bonds form is not because of the need to produce an “octet”, but rather because the bonded system of atoms is more stable (i.e., has a lower potential energy) than the unbonded system. Next, physical properties of simple materials are introduced (hydrogen, diamond, graphite, and metals) to illustrate how bonding and molecular-level interactions affect macroscopic properties. Students are introduced to 3D structures via physical and computer models, then to Lewis structures as simplified representations of these structures. Students learn to draw Lewis structures from molecular formulas and decode the information they contain, based on VSEPR, polarity considerations, and molecular shape. This enables students to determine the types of intermolecular forces present and their relative strengths; from these, students can—in theory, at least—predict the properties the substance will exhibit.

METHODS

Study Design

This study was performed at a southeastern research university, with students who were enrolled in general chemistry courses. All students involved signed informed consent and were notified of their rights as directed by the institutional review board. There are inherent conflicts of interest at play when researchers attempt to assess the impact of their own interventions, and we have attempted to minimize these effects by conducting assessments away from the lecture environment. All assessments were part of a laboratory assignment and were administered by researchers and teaching assistants who were not involved with the “lecture” aspects of the course. As far as the students knew they were completing a laboratory assignment, which is a separate course with a separate grade. Students were given credit for attempting to complete the assignments “in good faith”.

Over the course of a full year, students from two equivalent cohorts enrolled in general chemistry were asked to complete tasks outlined below. The treatment group ($N = 99$) consisted of students enrolled in the CLUE section, while the control group ($N = 127$) were enrolled in a concurrently taught traditional introductory general chemistry course. The control group was chosen from a total population of about 1400 students, such that they were equivalent to the CLUE group at the beginning of the Fall semester by SAT scores, major, sex, and TOLT scores (see the Supporting Information for details). During the second semester, only the students who took both first- and second-semester CLUE curriculum ($N = 56$) or who took both semesters of the traditional curriculum ($N = 83$), and who completed all the assignments used in the assessment,

were included for this study. It should also be noted that the “control” general chemistry course at this institution is “reformed”: that is, most instructors use interactive methods such as clickers, and group quizzes; learning objectives are defined; instructors meet weekly to discuss the material; and students complete online homework provided by the textbook publishers. However, the content of the control course is traditional in that a widely available text is used to provide the curriculum. The students take the American Chemical Society’s (ACS) general chemistry exam and typically score between the 70th and 75th national percentile; that is, when conventional assessments are used, students in the traditional curriculum appear to be quite accomplished.

Two areas were assessed: (i) students’ ability to construct Lewis structures; and (ii) their understanding of the purpose of Lewis structures; that is, the connection between structure and properties. We chose these two measures because of their importance. The ability to understand the information encoded within a representation begins with the construction of the structure. We contend that the ability to *construct* a structure is very different from the ability to *recognize* a structure, and that in fact, students who never need to draw structures (or diagrams or graphs) are missing an important part of their education.²⁰ Typically, students’ knowledge of Lewis structures is assessed using multiple-choice questions, and we have already shown that these students have great difficulty with this task when they must construct rather than recognize the structures.¹ Therefore, we chose to use OrganicPad, a tablet-PC based free-form structure drawing program that allows users to construct Lewis structures in a naturalistic way, using a pen and the tablet-PC interface, as our assessment instrument.²¹ The

students' actions as they draw the structure are recorded (and can be replayed) and the submissions are automatically graded as has been previously described.²² Students from both treatment and control groups were asked to draw several sets of structures, with differing difficulties, over the course of a full year of instruction (see the Supporting Information).

To ascertain whether students understand the purpose of Lewis structures, and the information that can be determined from them, we administered the Implicit Information from Lewis Structures Instrument (IILSI),⁶ a survey developed in our group and validated over the course of three years with over 8000 student responses. Students were asked to identify what information could be deduced from a Lewis structure and any other chemical knowledge that they may have (see the Supporting Information). During the last administration of the IILSI, students were also provided with a fairly complex Lewis structure (alanine), and asked to predict and explain any physical or chemical properties that the compound might have.

Students were evaluated at several points during the two semesters of general chemistry, as outlined below:

1. Preinstruction, to ensure that students in the treatment and control groups were not measurably different in their beginning abilities and knowledge.
2. After the first semester, to investigate whether the treatment had any effect (post-Fall semester).
3. Before the second semester, to investigate whether students had retained the skills and knowledge over the month break between semesters (beginning of Spring semester).
4. After the second semester to investigate whether students retained the skills and knowledge over the whole instructional year (post-Spring semester).

The studies on students' ability to construct Lewis structures and their understanding of the purpose of Lewis structures involve nonparametric analyses as the data are not normally distributed and are often dichotomous. The effect size or power effect for results that indicated a significant difference between the two groups or within a group was evaluated; χ^2 test results are reported using the phi coefficient (ϕ) while the Pearson's (r) coefficient is used for Mann–Whitney and Wilcoxon rank sign analyses. The statistical values for each of the measurements can be found in the Supporting Information.

RESULTS AND DISCUSSION

Development of Ability To Draw Lewis Structures

The two groups (CLUE and control) were found to be statistically equivalent in terms of their preinstruction ability to construct Lewis structures. The control group mean was 10% and treatment group mean was 14%; that is, neither group appeared to have had (or have retained) a great deal of prior knowledge about this task, even though all these students had taken at least one high school chemistry course. Over the course of the two-semester sequence, students completed four sets of Lewis structures using the OrganicPad interface. Figure 2 shows the average percentage correct, the p -value and effect size (r) for all 12 structures for both groups at the end of the Fall and Spring semesters, and also the average for the most difficult structures.

It is clear that even after the first semester the CLUE student cohort exhibited a significantly improved ability to construct Lewis structures, which became more pronounced when we looked at the more difficult questions—those that do not

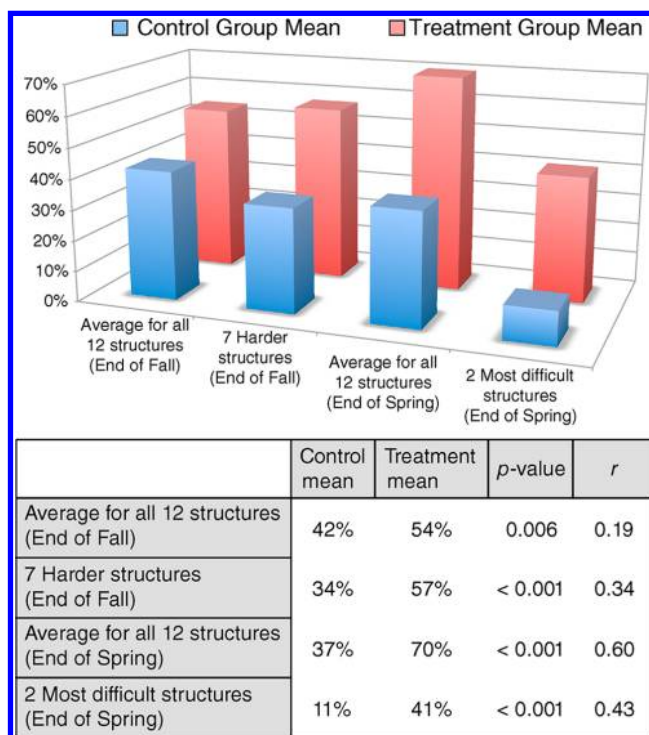


Figure 2. Percentage correct data for sets of structures at the end of each semester. The post-Fall administration results show a significant difference in the overall average: $U = 4358.5$; $Z = -2.75$; $p = 0.006$; $r = 0.19$; for the seven more difficult structures (ones that do not contain a central atom), $U = 3411.5$; $Z = -4.93$; $p < 0.001$; $r = 0.34$. By the post-Spring administration, the difference between the two groups had grown: $U = 691.0$; $Z = -7.10$; $p < 0.001$; $r = 0.60$; for the two even more difficult structures, $U = 1348.0$; $Z = -5.05$; $p < 0.001$; $r = 0.43$.

contain a central atom (i.e., the majority of structures that students would encounter in their future studies). After the second semester, the difference between the two groups had grown larger; for 11 of the 12 structures, the two groups were significantly different. Therefore, it was not surprising that a significant difference was found for the overall success rate between the two groups: $U = 691.0$; $Z = -7.10$; $p < 0.001$; $r = 0.60$. The effect size of 0.60 is classified as "large".²³ One unfamiliar chemical formula (C_3H_7NO), and one that had proved difficult earlier ($C_4H_8O_2$), were included in the post-Spring semester administration to investigate whether students can transfer their knowledge to unfamiliar situations. To our knowledge, the first structure had not been introduced in either lecture or lab for any of the students. A significant difference emerged in the success rate for these two structures between the control and treatment groups ($U = 1348.0$; $Z = -5.05$; $p < 0.001$; $r = 0.43$). Very few students in the control group could draw a reasonable structure for either of these compounds. It should be noted, however, that even in the CLUE treatment group, only 40% of the students were successful. The use of knowledge in unfamiliar situations is an important outcome for education, but one that remains quite elusive.

For each administration of the 12-structure set, six of the structures were the same, and the other six were changed each time. In this way, we were able to investigate whether familiarity with the structures improved student success, and also to look at new and unfamiliar structures. Figure 3 shows how the students' success rates changed on the six structures that were

on both administrations (post-Fall semester and end of the Spring semester).

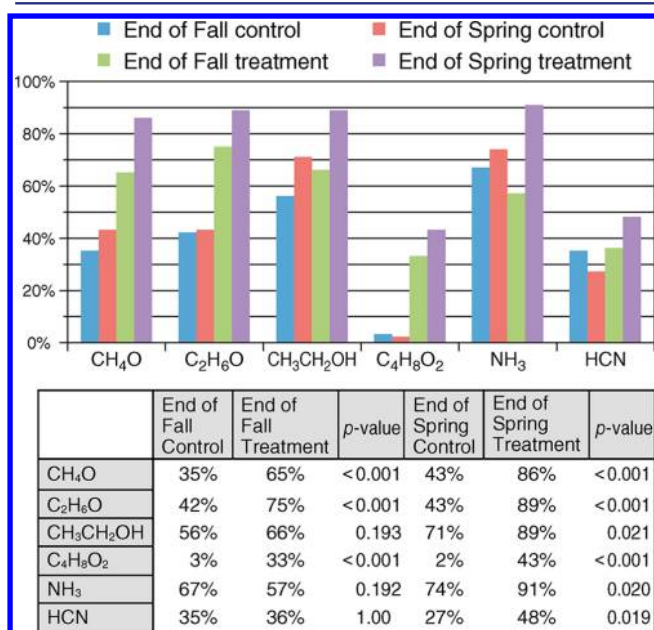


Figure 3. Success rates for control and treatment groups on the six structures that were administered both post-Fall and post-Spring semester.

Comparisons *within* the control group indicate that there was no significant difference between their end of the first-semester to end of the second-semester assessment scores. The treatment group, however, performed significantly better at the end of the second semester (compared to the end of the first semester) on three of these six structures. That is, the CLUE students continued to improve over the course of the second semester, while the control students remained static. By the end of the second semester, the CLUE students significantly outperformed the control cohort on every structure, even for HCN, NH₃, and CH₃CH₂OH, for which the performance had been equivalent after the first semester. We believe that the lack of improvement in the control students may be attributed to the traditional curriculum structure, in which blocks of material are treated as discrete “chunks” (chapters) and rarely presented in terms of how these topics relate to each other. So, even though the students take a cumulative final examination (ACS General Chemistry Exam),²⁴ which requires students to review two semesters’ worth of material, it seems that reviewing for a multiple-choice final exam is not sufficient to enhance or even retain these skills (which are crucial for the next course in the sequence, organic chemistry).

Development of Ability To Use Lewis Structures To Make Inferences about Properties

The ILSI was used to identify what types of information students believed they could deduce from a Lewis structure, as well as any other chemical knowledge they might have had. Both groups were able to indicate (not surprisingly) that structural information could be determined. After the first semester of instruction, significant differences emerged in items that correspond to physical or chemical properties, and although some of these gaps narrowed after the second

semester, a significant difference still existed among six of the choices for treatment and control groups.

Most of these choices referred to items that might be classified as physical or chemical properties. Interestingly, the answers “relative boiling point” and “relative melting point” were statistically equivalent for the two groups, whereas “physical properties” was significantly different ($p = 0.003$, $\phi = 0.25$) (Figure 4). That is, some students from the control

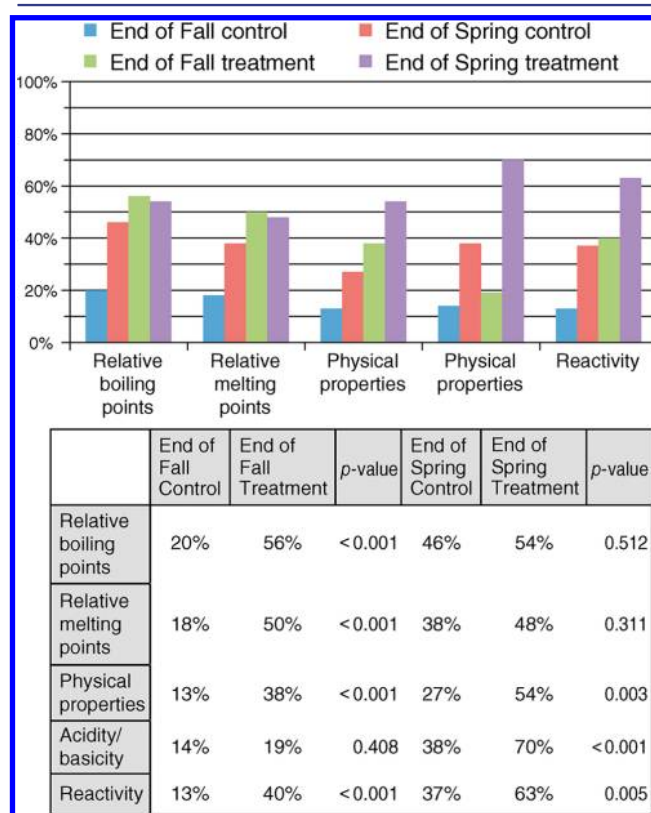


Figure 4. ILSI information that can be determined from a Lewis structure, reported post-Fall and post-Spring semester for treatment and control groups.

group chose melting and boiling points, but *not* physical properties. We believe this may be because, in the traditional curriculum, students are explicitly asked to rank the relative melting or boiling points of substances when given their structures. However, fewer students in the control group were able to make the more general connection with physical properties, which requires another level of abstraction. Talanquer⁵ has reported a number of examples in which students were able to use heuristics to predict answers to questions, while not fully understanding the underlying principles.

We also found significant differences between CLUE and control groups in their understanding of chemical properties: reactivity ($p = 0.005$, $\phi = 0.24$) and acidity–basicity ($p < 0.001$, $\phi = 0.30$). That is, CLUE students appear to have a better understanding of the uses of and information that is encoded into a Lewis structure. As students completed the ILSI survey at the end of the second semester, they were also asked to predict what properties a fairly complex structure (alanine) might exhibit, and provide explanations for their predictions. Of CLUE students, 51% recognized and reasoned that the substance had either or both acidic and basic properties,

while only 23% of the control students made this connection ($p < 0.001$, $\phi = 0.30$).

We are currently following these students as they move through organic chemistry, to see whether their improved skills transfer into an increased ability in a course in which the structure–function connection is even more important.

Instructor Effect

Over the years, many instructional innovations have appeared (initially) to be effective; however, it has proven difficult to distinguish the effects of the instructor from the effect of the curriculum. Clearly, one approach would be for one instructor to teach two sections of the same course, with an identical cohort of students. However, while this might be the “gold standard” of educational assessment, it is generally impractical and problematic in theory, because it assumes that the instructor is an unbiased actor within the experiment, something unlikely to be the case. We chose to assess the instructor efficacy by using data from a prior semester when the same instructor taught a traditional section of general chemistry (using traditional materials). Students in the instructors’ section were compared with an equivalent cohort from all the other sections using the same measures (SAT scores, major, sex, and TOLT). No significant differences were observed between the two groups of students in their ability to construct Lewis structures. (See the Supporting Information.) That is, students who took general chemistry from the CLUE instructor in an earlier semester using the traditional curriculum *did not perform better than their peers*.

CONCLUSIONS

The two main findings of this study can be synopsized as follows. First, students in the CLUE curriculum showed significantly improved abilities to draw Lewis structures compared to a cohort of students who took a more traditional general chemistry curriculum. This effect increased over the course of the two-semester CLUE sequence and the effect size can be classified as large. A sizable part of the CLUE-associated improvement comes from the ability of students to construct relatively complex structures, *including structures that the students have not seen before*.

Second, CLUE students showed a significant improvement in their understanding of the types of information that are implicitly encoded within a Lewis structure, when compared to the traditional student cohort in the control group. That is, CLUE students had a better understanding of the purpose of Lewis structures.

We believe that these improvements stem from the research-based, scaffolded structure of the CLUE curriculum, rather than any inherent ability in the instructor, as the same instructors’ students did not show such differences when using a more traditional curriculum, even while using “best practices” for teaching large enrollment courses. The CLUE learning progression from structure to function was deliberately designed to help students develop appropriate prior understandings (e.g., about bonding and three-dimensional structures); new material was explicitly linked to this prior knowledge, and explicitly connected at each further step to material students had already learned and material that they were about to learn. Students were given a reason why they needed to learn this material, and therefore, many of them were able to learn more meaningfully.²⁵

Assuming that a major goal of education is (or should be) to provide students with the tools needed to apply their knowledge effectively in new situations, the improvements observed using the CLUE curriculum are especially promising. The majority of the CLUE-associated improvements involve students’ abilities to draw quite complex structures, especially ones with which they are unfamiliar.

Implications for Teaching

The evidence presented here suggests that the CLUE curriculum and materials can produce more robust learning in students with that learning becoming transferrable to more complex situations. For those who are unable (or unwilling) to embark upon a complete reform of the general chemistry course, it may be, at least in this instance, that coherent learning progression design could and should be incorporated into a more traditional approach, by taking care to teach the material in a way that makes the links between structure and properties explicit. It is important to remember that difficult, and nonintuitive concepts such as the relationship between molecular structure and macroscopic properties take time to develop, and that an awareness of how difficult many of these tasks are for beginning students needs to be explicitly acknowledged. That said, structure–property relationships are just one of a number of complex scientific constructs that students find difficult to master. Our observations suggest that appropriately designed learning materials should be explicit in addressing the often deeply counterintuitive nature of scientific ideas, the sequence of concepts that must be learned, the time it takes to learn them, and the kinds of activities that lead to robust learning to help students learn and transfer their knowledge to new situations.

Limitations of the Study

While these findings are promising, we are aware that, as in the case with science in general, replication is necessary to provide both substantiation and clarification of limitations. Different learning environments with different instructors could reasonably be expected to produce different outcomes, and extensive field studies are essential to determine best practices in chemistry course and curricular design, delivery, and learning assessment. What seems well established, however, is that merely changing the way a traditional curriculum is presented is not enough to bring about the robust learning; the curriculum itself must also be redesigned.

ASSOCIATED CONTENT

Supporting Information

Study design details; IILSI examples; statistical analyses and data. This material is available via the Internet at <http://pubs.acs.org>.

AUTHOR INFORMATION

Corresponding Author

*E-mail: cmelani@clemsun.edu

Notes

The authors declare no competing financial interest.

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