Use of Simulations and Screencasts to Increase Student Understanding of Energy Concepts in Bonding

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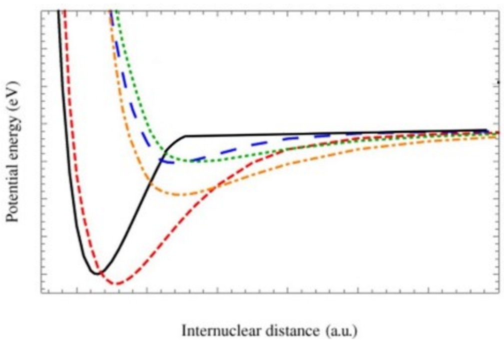
ABSTRACT

The growing popularity of flipped, blended, and online learning, combined with the need to support a student population with increasingly diverse backgrounds has led to the development and use of online materials to support students' learning of chemistry outside of a face-to-face classroom. Chemistry simulations provide opportunities to make such materials more interactive; however, it is important to understand how to best employ them to support students' independent learning outside of the classroom. The larger ChemSims project aims to determine how screencasts and simulations can be used to best support the development of students' conceptual understanding of core chemistry concepts in such environments. This paper focuses specifically on the concepts of force and energy as they pertain to bonding and intermolecular attractions. It describes the investigation of students' out-of-class use of a PhET simulation that illustrates force and energy changes that occur when two atoms come together or are separated. As an introduction to bonding, students completed out-of-class assignment questions in one of three different treatment conditions: (1) exploring the simulation directly using guided instructions; (2) watching an expert-narrated screencast using the same simulation; or (3) watching an "enhanced screencast", consisting of the expert-narrated screencast plus additional information related to the formation and breaking of bonds in chemical reactions. Comparing scores on pretest and follow-up questions indicated that all treatments resulted in small

learning gains with some learning objectives indicating greater gains than others. Further, findings indicate that the enhanced screencast was able to help student better connect this concept to the phenomena of ATP hydrolysis. Finally, using eye tracking to contrast student use of the simulation as compared to the screencast in completing the assignment suggests that, while the screencast may not result in increased conceptual gains, it may serve to make the assignment seem easier than if students are required to engage with the simulation themselves to work through the initial questions.

GRAPHICAL ABSTRACT



KEYWORDS

High School / Introductory Chemistry, First-Year Undergraduate / General, Chemical Education Research, Computer-Based Learning, Distance Learning / Self Instruction, Internet / Web-Based Learning, Multimedia-Based Learning, Problem Solving / Decision Making, Atomic Properties / Structure, Noncovalent Interactions

INTRODUCTION

Given the increased use of flipped, blended, and online learning it is important to understand how to effectively design and use materials for use in these environments. One challenge is to design materials that provide students with opportunities to actively engage with the content; something research has identified as essential for development of conceptual understanding.[1] The use of simulations in chemistry courses has become more frequent and using them outside of the classroom in an online environment is one mechanism to provide active engagement with concept development at the atomic-molecular level. One benefit to such use is that the time devoted to the activity is not defined by the instructor/class length but rather by the individual students based on their needs.

However, it is unlikely, particularly with difficult concepts, that students will be able to identify the appropriate patterns or make desired connections without some level of scaffolding to direct their interactions with the simulation.[2,3] Further, even with scaffolding, there is evidence that students may still not focus on the desired patterns or interactions or may incorrectly interpret what they are seeing.[4,5] In this case, a screencast where an instructor is able to explicitly focus students' attention may address some of these issues. The larger ChemSims project[6] aims to identify how simulations and screencasts can be used to support student development of particulate level understanding of core chemistry concepts. This paper focuses on the development and study of materials related to supporting students in building a conceptual understanding of potential energy as it relates to the attraction and repulsion between particles at the atomic-molecular level.

The interactions of matter and energy are foundational to chemistry. In particular, understanding energy changes at the atomic-molecular level as they relate to the processes of breaking and forming bonds or attractive forces between atoms and molecules is crucial to understanding the macroscopic energy changes associated with chemical process, including those in biological systems. Yet student understanding of potential energy at the atomic molecular level is generally not stable or normative,[7] rather ideas are frequently applied inconsistently or non-productively, particularly in terms of energy as it relates to bond breaking and forming.[8–10] One suggested mechanism for addressing this is more explicit attention to the role of potential energy as it relates to energy changes at the atomic-molecular level.[7,11]

Difficulties with Potential Energy

One particular issue with students' understanding of energy at the atomic-molecular level is use of the unproductive idea that that breaking bonds releases energy.[8–10] Research has shown that even after instruction, about half of students still frequently apply the idea that bond breaking releases energy,[8,12] and that even some graduate students retain this non-productive idea.[12] Cooper and Klymkowski[11] suggest that there are three major sources that contribute to students' difficulties in understanding of energy at the atomic-molecular level, particularly as it pertains to bond breaking and forming. First, students are exposed to the concept of energy in everyday life as they learn about food as energy and see energy labels on food packaging, or encounter burning fuels as a means for energy production. This idea of energy storage in food or fuels is reinforced by biology instruction that teaches them about metabolism as a process that breaks down food and releases energy or portrays ATP as a molecule with a "high-energy bond." Second, students learn about energy in physics from a macroscopic perspective, the most common example being the conversion between potential and kinetic energy during processes such as a ball rolling down a hill. In traditional physics instruction, there is no requirement for students to make connections to energy at the atomic or molecular level. Finally, chemistry textbooks and instruction typically do a poor job, if any, of making explicit connections between physics (the macroscopic examples of potential and kinetic energy that students are familiar with) and interactions of atoms and molecules. Nor do they typically make explicit the connections between familiar biological processes, such as the breakdown of glucose into carbon dioxide and water in metabolism, and the changes in potential energy interactions of the reactants and products. Given the very different ways that energy is taught in these different science disciplines and the lack of connection between them, it is not surprising that students frequently lack a coherent, stable, and normative understanding of energy and struggle with this concept.[13]

In learning about energy from multiple, unconnected perspectives it is understandable that students may apply different knowledge fragments based on the situational context. This is consistent with DiSessa's "knowledge in pieces" framework.[14] In this view, learning is viewed from a constructivist perspective, where initial knowledge is often fluid and unstable, starting with intuitive knowledge (which DiSessa calls p-prims) and other smaller-grained knowledge elements being activated by particular contexts. Through the learning process new knowledge elements are acquired and knowledge is reorganized to develop more mature concepts that are more stable and normative,[15] and applied more consistently across different contexts or conditions. Until a student has been able to pull such pieces together into a more stable and coherent understanding, smaller factors in the context of an individual question may activate knowledge fragments that are not productive in constructing a scientifically accurate explanation.

Difficulties in Interpretation of Graphical Representations

Another factor that may hinder students' understanding of PE at the atomic-molecular level is their ability to correctly interpret PE well diagrams or graphs. Scientists frequently use graphs to summarize data in a concise manner to visualize trends and make sense of the data. As a result, students in introductory chemistry courses are expected to construct and interpret graphs. Yet, students often struggle with these tasks. Students find carrying out function tasks most difficult when data was presented as a graph, as compared to using a table or augmented bar chart.[16] Additionally, chemistry and math students have been shown to successfully solve algebraic problems, yet face difficulty constructing a related graph.[17] These results suggest that the difficulty was the translation of the algebraic relationship to the construction of a graph as opposed to an issue with the content.

Of particular interest to this study is the findings regarding student difficulties in interpreting and using potential energy well graphs to reason about total, kinetic, and potential energy in physics.[18] They found that one of the main difficulties that students had was with negative potential energy values, many students believing that potential energy cannot be negative. Separately, an examination of student reasoning about the potential energy between two charged blocks showed that after interactive instruction, students were largely able to correctly answer questions about PE change when two blocks of the same charge were pushed together (it increases), but fewer than half of the student correctly answered the question about change in PE when two blocks of opposite charge were pushed apart (it increases).[19] Student interviews indicated that many students were applying the idea that potential energy had to scale with the strength of the attractive force between the objects. This is consistent with DiSessa's[20] p-prims or Talanquer's[21] heuristics which can be defined as intuitive knowledge that serve as shortcut reasoning strategies. In the PE case, students appear to be frequently accessing the idea that more implies more.

Visualizations in Chemistry and Cognitive Load

Simulations can help address the difficulties students have in integrating the particulate level with macroscopic and symbolic representations by helping them visualize the invisible.[3,22–25] Employing such visualizations can reduce cognitive load for the learner by making connections between representation levels more overt and easier to access. Further, dynamic representations, such as animations and simulations, make the interactive nature of chemistry more explicit, helping students understand the crucial interactions between particles. Finally, allowing students to interact with visualizations, such as through the use of a simulation, has been demonstrated to increase concept learning and transfer, by increasing engagement in the learning process.[26]

Careful thought, however, must go into the design of materials that support student use of simulations outside of the classroom. Well-designed materials will provide scaffolding that guides students in manipulating the simulation in ways that produce productive observations. This serves to minimize the extraneous cognitive load associated with learning how to best manipulate the simulation conditions to construct conceptual understanding. This extraneous load is the cognitive demand introduced by the delivery method of the content, as opposed to the intrinsic load or difficulty of the content itself. The materials developed as part of the ChemSims project aim to reduce the extraneous load by providing scaffolded instructions for the use of the simulation as well as question prompts to help students identify important patterns and make connections between the different simulation elements.

While simulations may allow direct interaction with material, their design does not necessarily allow for the removal of all extraneous material or the highlighting of crucial information in order to help students organize their mental models and make the best learning gains possible. One way to further aid individuals in learning is the use of audio narration alongside images.[27] Therefore, it is possible that screencasts, which pair expert-guided narration with manipulation of a dynamic simulation, may significantly decrease cognitive load and increase student learning of difficult concepts. Differences in cognitive load may then influence how students approach and complete a given activity. Previous work looking at the concepts of solubility and kinetics indicates that screencasts may result in greater learning gains,[28] greater attention on the electronic resource,[28] and differing amounts of perceived and actual time on task.[29] This paper aims to investigate the use of simulations alone, versus the use of simulations incorporated into screencasts, for the teaching and learning of energy changes at the atomic-molecular level.

Research Questions

This study was conducted to address the following research questions:

1. What are the impacts of outside-of-class usage of simulations or screencasts on students' conceptual understanding energy changes at the atomic-molecular level?

2. How can a screencast be most effectively used to aid student learning outside of class?
3. How and where do students allocate attention when using a guided assignment coupled to either a simulation or screencast?

METHODS

Developing effective scaffolding to reduce cognitive load and support student use of simulations outside of class requires careful consideration that is best accomplished through an iterative design and evaluation process. The overarching iterative design framework used for this study is based on Wiggins et al.[30] and illustrated in Figure 1.

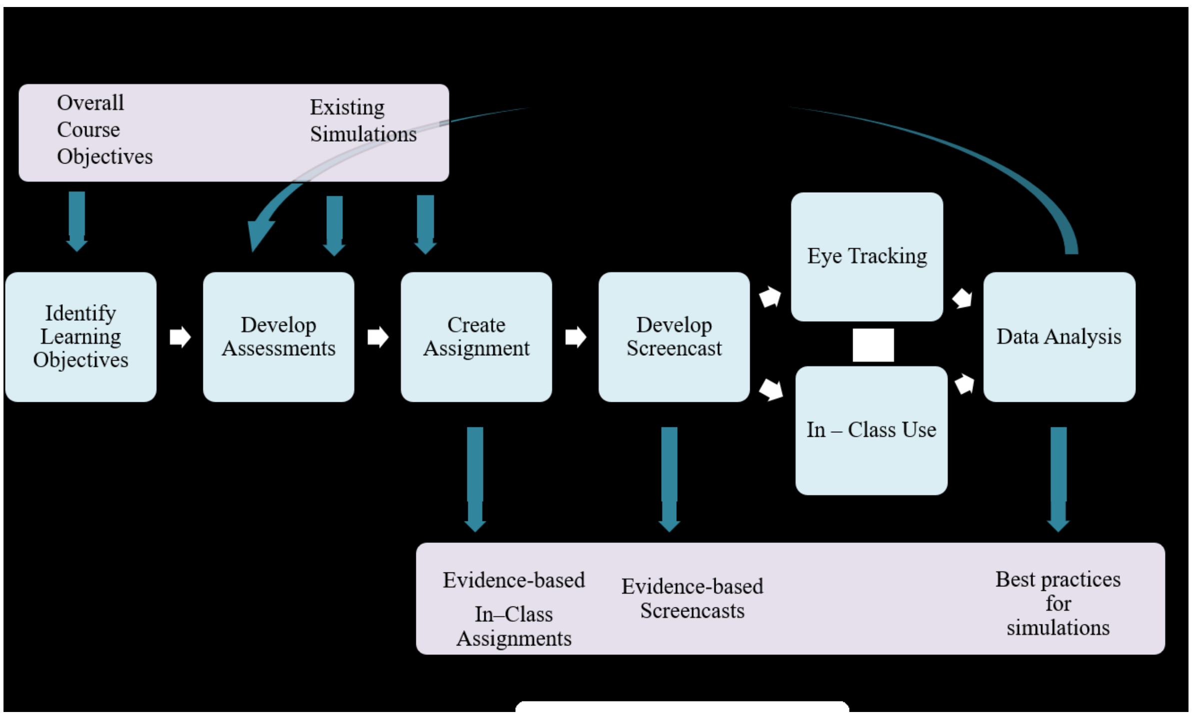


Figure 1. Design process illustrating the creation of learning materials from course objectives and revising them based on previous iterations.

The collection of pretest and matched follow-up question data allows for a quantitative measure of student learning which can shed light on research questions 1 and 2. Further, qualitative analysis of student written responses, both to the pre/follow-up questions as well as the assignment questions, can provide evidence to support the revision of instructional and assessment materials through this iterative design model. For example, reviewing student responses to a question asking them to apply what they learned about the energetics associated with bond breaking and forming to ATP hydrolysis led to the development of an enhanced screencast that supplemented the simulation with additional illustrations and narrative that connected the energetics students investigated using the PhET simulation[31] with a chemical reaction (described in more detail in the Enhanced Screencast section). Finally, eye-tracking data can provide insight into how students are using the simulation and screencasts resources (research question 3) by providing a measure of how students allocate their time when engaging with the visual representations. The following sections describe in more detail the materials and their development as well as the data collection and analysis procedures.

Simulation

The bonding and interactions between atoms at the particulate level are critical to understanding macroscopic energy changes during reactions; representing these interactions symbolically and graphically is common in general chemistry. Because of the importance of understanding energy changes at multiple levels of representation, an appropriate simulation incorporates multiple levels and helps students make connections between them. The PhET Atomic Interactions simulation[31] was identified as an effective resource for helping students learn about bonding and interactions between particles (Figure 2). This simulation provides multiple representations, including graphical and particulate diagrams, and allows students control over crucial features such as particle identity and spacing. Specifically, this simulation contains the following features deemed critical:

- Selection of different atom pairs, where some pairs have only London dispersion forces between them, and other atom pairs will bond covalently. In each pair, one atom can be moved by the user to change the distance between the atoms in the pair.
- Arrows showing the total force between the atoms as well as the component forces.
- Graph showing how potential energy varies as a function of distance between atoms.

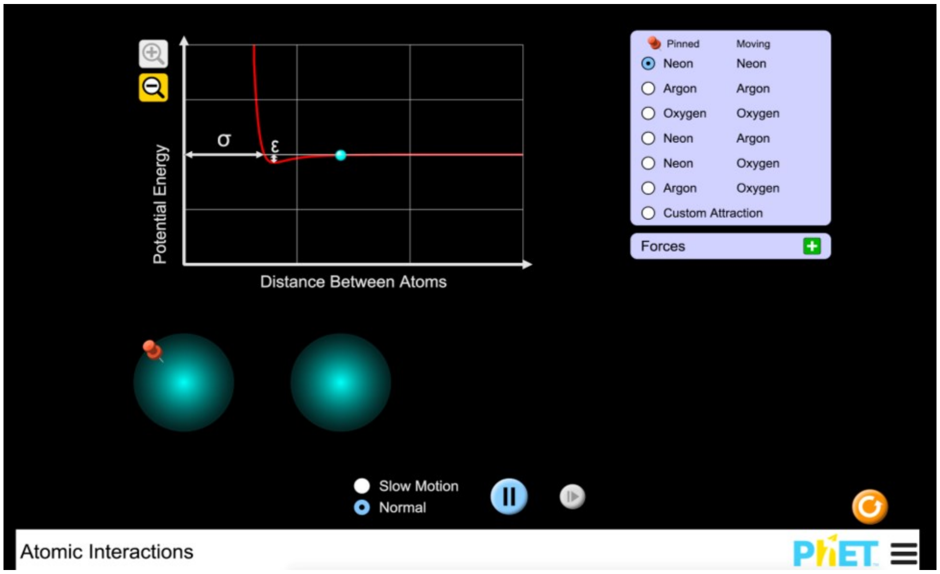


Figure 2. Screenshot of PhET Atomic Interactions simulation. *Simulation image by PhET Interactive Simulations, University of Colorado Boulder, licensed under CC-BY 4.0* (Atomic Interactions, n.d.)

A particular strength of this simulation is that by changing the distance between the atoms, users can immediately and directly see how the potential energy changes on the graph. However, while the simulation makes strong connections between the particulate and graphical levels, it does not reference the macroscopic level or changes in energy that occur on this level (i.e. net endo-/exothermic as energy is absorbed or released from the system).

Materials Creation

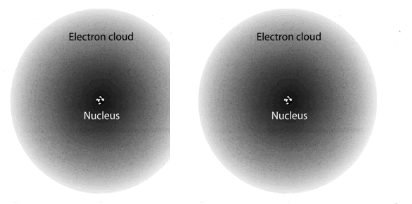
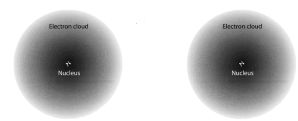
Using the design approach outlined in Figure 1, the following key learning objectives related to atomic interactions were identified:

1. Explain how subatomic particles lead to attractions between two atoms
2. Use potential energy to explain the energy changes associated with the breaking and forming of covalent bonds and intermolecular forces
3. Explain how both strength of interaction and distance between interacting atoms are represented on potential energy well diagrams

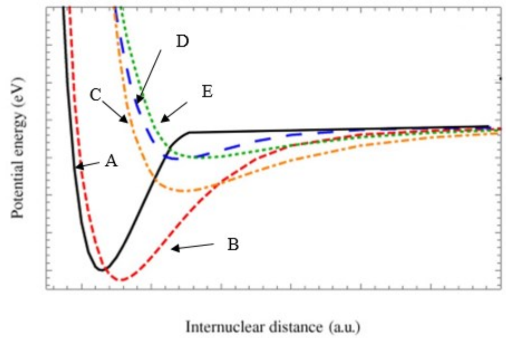
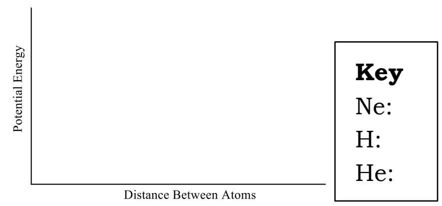
A set of five assessment pretest and matched follow-up/assignment question items were identified to measure student progress towards the desired learning goals. As this activity was designed as an introduction to the concept of PE and attraction/repulsion between atoms, students had not received any formal in class instruction prior to completing the pretest and assignment. Yet, as students enter our classes with varying levels of prior knowledge it was important to acknowledge and assess for this. The pretest consisted primarily of multiple-choice questions. Three of these questions (Table 1 questions 2-4) were developed as part of a Masters project assessing conceptual understanding of atomic structure, covalent bonding, and bond energy.[12] The other two questions were designed to "match" the assignment/follow-up questions as shown in Table 1. In an ideal world, we would be able to interview students, ask students more questions, or have students construct explanations on the pretest; however, as these materials are designed primarily as instructional tools, using a pretest that takes students more than ten minutes to complete was not possible. Further, we acknowledge that multiple-choice questions can overestimate student understanding[32,33] and that constructed responses provide opportunities for students to provide reasoning to help us better assess the underlying mental models or concepts they are using. In this case, given the more fragmented mental models that students have relating to this topic and that it is often not explicitly taught in college chemistry courses,[11] it made more sense to use primarily multiple choice questions for the pretest rather than constructed response questions. In our previous work on other topics we have found that students are more likely to leave pretest constructed response questions blank or not engage with them meaningfully, whereas with multiple choice questions they are generally willing to select an option that appears to be consistent with their understanding. Employing a constructed response format in the assignment and as follow-up questions provides an opportunities for students to thoughtfully engage with the content as evidenced by their explanations and allows us to capture their reasoning.

The assignment consisted of guiding instructions and questions designed to scaffold students' use of the simulation and learning of key concepts, plus the follow-up questions to assess student understanding. These materials were tested and revised based on student responses in order to clarify questions or modify scaffolding where students were less successful at making the desired connections. After three cycles of student use and revisions, the assignment used to collect the data in this study was finalized (final versions of the pretest and assignments are included in supporting online materials).

Table 1. Matched Pretest and Follow-up assessment questions with corresponding learning objectives.

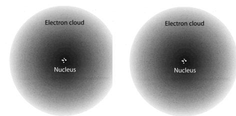
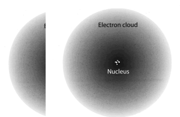
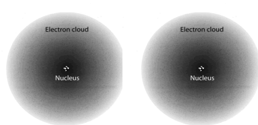
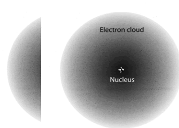
Learning Objective	**Pretest**	**Follow-up (F)/Assignment (A) /Summary (S) Questions**
1	1. Below is a picture of 2 Hydrogen atoms:  a. Describe what you think will happen: I. They will attract each other and start moving towards each other II. They will repel each other and start moving away from each other III. They do not interact at all b. Explain your reasoning for part a.	F1. If you have two atoms at some distance from each other as shown below, would you expect them to: (circle one) *attract each other* *repel each other*  What causes the attraction/repulsion?
1	2. If two H atoms are already bonded together, what happens at the molecular level if you try pushing the atoms closer? a. The nuclei will repel from each other; however, the electrons will not repel from each other since they need each other to make the orbital full. b. The electrons become closer and the bond between them becomes stronger. The force between the electrons can hold the atoms together better. c. The nuclei will repel from each other even more and the resulting net orbital will become more spherical. The electrons move around to the side of the nuclei. d. The potential energy increases to form bond energy. The bond energy is needed to hold atoms together. e. Both the electrons and nuclei repel each other. The potential energy increases and the bond becomes less stable.	A2: If you start at the bottom of the PE well and push the atoms together, does this require an input of energy or a removal of energy? Justify your answer with evidence from the graph. A5: What interactions <u>between</u> the two neon atoms results in repulsive forces?

2	3. What happens when a bond is formed between two H atoms? a. The electrons of the two hydrogen atoms are attracted to each other because electrons like to be paired up, thus holding the two atoms together. b. A single bond is formed by the electrons making a solid connection between the two hydrogen atoms, like a stick joining the two atoms together. c. As the electron of one atom approaches the nucleus of the other, energy is transferred from the electron to the nucleus which forms the bond. d. As the hydrogen atoms move closer together, there is an attraction between each electron and the nucleus of each hydrogen atom making the two hydrogen atoms stick together.	F3: As indicated above, 2 H atoms come together to form a covalent bond. Describe what causes the attractive forces that hold the 2 H atoms together.
2	4. Which of the following statements accurately describes the energy changes during bond formation and breaking? a. Energy is released as heat during bond breaking although energy is required to keep bonds in place. b. If a reaction is exothermic the bonds that are broken release energy to the surroundings. c. The energy that is required to break bonds is equal in magnitude to the energy released when bonds are formed, because energy can neither be created nor destroyed. d. When bonds are broken energy must be absorbed by the system, but when bonds are formed energy is released.	S1: **Claim:** Given that we know energy is not created or destroyed, when atoms come together from a large distance, energy is (circle one)… *Absorbed* *Released* **Evidence:** What evidence from the graph(s) supports your claim? **Reasoning:** Explain why the evidence from the graph supports your claim. S3: **Claim:** To break a bond or a London Dispersion force (pulling atoms apart), energy is: (circle one) *Absorbed* *released* *initially absorbed and then released* **Evidence:** What evidence from the graph(s) supports your claim? **Reasoning:** Explain why the evidence from the graph supports your claim.

3	5. Below is a graph of potential energy (PE) as a function of the distance between two atoms.  a. Which of the curves (A through E) shows the strongest interaction between two atoms? b. What made you choose that curve for part a? c. Consider just curves A and C. If one curve depicts the interaction that results in a covalent bond and one depicts the interaction for London Dispersion Forces, which curve would depict the covalent bond? (circle one) Curve A Curve C d. Explain why you chose that curve for part c.	F1. Sketch the shape of the potential energy vs. distance between atoms graph depicting the interaction between two Ne atoms in the space below.  Using different colored writing implements or different line styles (dotted or dashed), add the potential energy curves for (1) 2 He atoms and (2) 2 H atoms to the graph. Be sure to indicate which is which in the "Key" box above. *Note: you will not find either of these in the simulation but you should consider the following in drawing your curves.* a. He atoms form London Dispersion attractions b. H atoms form a covalent bond c. He (Z=2) and H (Z=1) are similar in size and smaller than Ne (Z=10) Based on the above information, in drawing your curves be sure to correctly illustrate the relative optimum distances and the relative depths of the PE wells.

Using the assignment instructions and questions as a guide, a screencast was created; this was an expert led video demonstrating the simulation and suitably pausing to allow for the students to complete the assignment questions.[34] The goal of the screencast was to potentially reduce students' cognitive load, however the screencast was intentionally designed to be a parallel treatment to the simulation--that is, students answered the same or similar questions by watching the screencast video rather than interacting with the simulation directly. Additionally, the screencast narration highlighted key aspects of the simulation and focused on critical features of the graphical and particulate representations in order to guide attention and potentially lower cognitive load for students, but did not provide any additional information the simulation students would not have. No direct answers were given for the questions included in the guided assignment for either the screencast or simulation students. Both the simulation and screencast assignments were designed to allow students to grapple with the conceptual understanding and sense-making on their own. An example of the match between screencast and simulation assignments is shown in Table 2.

Table 2. Simulation and screencast assignment prompts and accompanying narration.

Simulation Assignment	Click on the pause button. Click on ✚ sign beside <u>Forces</u> and then click the radial button beside total force. Again, drag the unpinned Ne atom so that atoms are in the position shown below.  **What do you notice about the [illegible]es between the two atoms?** (*You may have to move the unpinned Ne slowly towards the other Ne atom to see this*.) **Does this represent attraction or repulsion between the two atoms?** Drag the unpinned Ne atom so that the atoms are in the position shown below. **What do you notice about the direction of the forces between the two atoms?** **Does this represent attraction or repulsion?** 
Screencast Assignment	What do you notice about the direction of the total force between the two neon atoms when they are in the position shown below? Does this represent attraction or repulsion between the two atoms?  What do you notice about the direction of the total force between the two neon atoms when they are in the position shown below? Does this represent attraction or repulsion between the two atoms? 
Screencast Narration	The simulation allows us to view the forces at play when these atoms interact. The green arrows represent the total forces present in this situation when the atoms are far apart from each other. [arrows appear on screen] Do these arrows represent an attractive or repulsive force? Take a second to answer this question on your worksheet. Now we'll take a look at what happens when the two atoms are very close to each other and are overlapping. Looking at the green arrows is there now an attractive or repulsive force? Take a second to answer the question on your worksheet.

Enhanced Screencast

Upon being asked about energy changes within the context of a chemical reaction, many gave responses that were inconsistent with those they gave when asked about energy changes within the context of particles coming together or moving apart. To try and help students develop a mental model that was more coherent and thus more consistently applied across concepts, an enhanced screencast was developed. The original screencast was intentionally designed to parallel the experience of the students directly interacting with the simulation. However, screencasts have the potential to include additional elements to support student learning. To explore this potential, an enhanced screencast consisting of the original, fully parallel screencast described above and an additional two-minute segment illustrating the particulate level energy changes associated with the combustion of methane was developed and administered to a group of students.[35] This addition was designed to help students make the connection between what they observe regarding potential energy in the simulation and how that relates to the energy changes associated with bond breaking/forming in a chemical reaction. Ideally, this would help the students develop a more coherent understanding of energy that they can meaningfully apply in both chemistry and biological contexts. The additional segment was not based on the PhET simulation and instead created in Microsoft PowerPoint, illustrating both visually and with explicit narration that energy must be added to break bonds in the reactants, but is released when new bonds in the product molecules are formed, resulting in an overall release of energy. It was added to the original screencast video using Camtasia.[36]

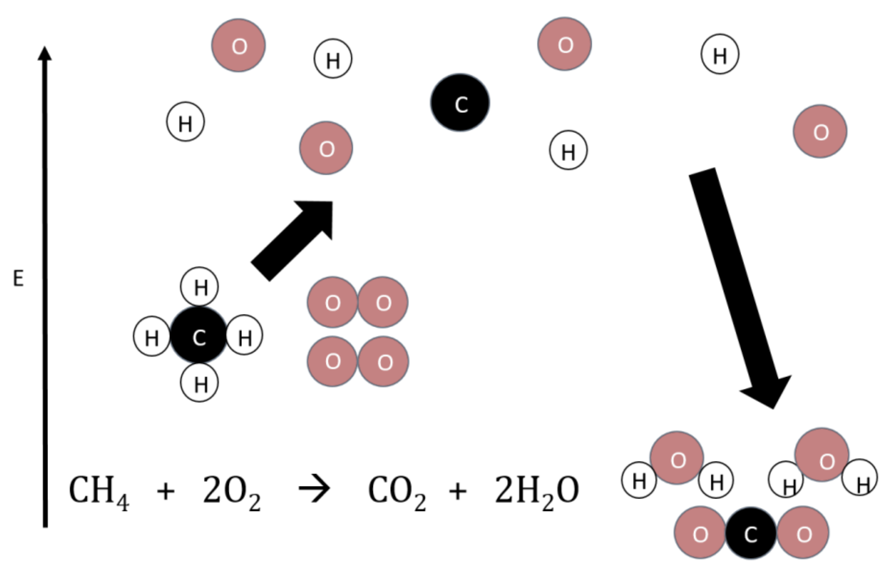


Figure 3. Image from the enhanced screencast depicting the energy changes associated with the combustion of methane.

To investigate the impact of this enhanced screencast treatment, an additional application question asking students to describe the energy changes during the hydrolysis of ATP in metabolism was added to the follow-up questions. Although there was no matching pretest question, this question was designed to determine if students would provide consistent answers for the summary questions related to bond breaking and formation (Table 1 questions S1 and S2) and a question that was situated in a real-world phenomenon. ATP was chosen for this question as a familiar biological example, and one where students often apply the nonnormative idea that breaking bonds releases energy.[9] All three treatments were designed to help students make the connection between energy and bond breaking/forming, but only students in the enhanced screencast treatment saw the added combustion example that provided an example of this in the context of a chemical reaction.

Classroom Study: Participants and Study Design

This study was reviewed and approved as exempt by the Institutional Review Boards (GVSU Ref. No. 16-012-H; MSU x15-799e). The participants were drawn from undergraduate students in General Chemistry 1 at two large public institutions in the midwestern United States. Student data was collected and used to guide revisions to the assignments three times, as was outlined in Figure 1. The data analysis presented here focuses on the final iterations of the assignment and the responses of those students. Table 3 shows the number of participants who consented to this study for each treatment and institution.

Table 3. Participants in the research study from each institution and in each treatment group.

Treatment	Institution 1	Institution 2	Total
Simulation	41	51	92
Screencast	58	65	123
Enhanced Screencast	87	--	87

In order to test these treatments, students first completed the pretest, and were then assigned to use the simulation, screencast, or enhanced screencast to complete the assignment. After working through the assignment, all students were given the opportunity to use the screencast to answer the "Going Further" questions, regardless of their initial treatment. Finally, all students completed the Follow-up questions, including the additional application question, and were allowed to use the simulation as needed. A diagram of this treatment scheme is shown in Figure 4.

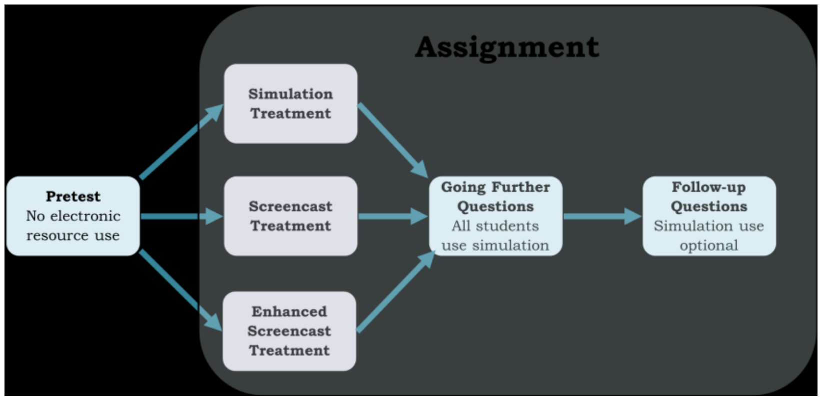


Figure 4: Experimental design for classroom study.

Responses to the constructed response questions were coded using the coding scheme provided in the Supporting Information. Codes for each question were developed during the first iteration of the materials and then revised for subsequent iterations where questions were modified. In developing the initial coding scheme, we used an inductive approach where two researchers each took a set of about 75 responses and identified common themes in the student answers for each of the questions, also noting the approximate frequency of the themes. The researchers then compared the themes for each question and came to consensus regarding common themes, or codes, for each question. The researchers then swapped data sets and applied the coding scheme deductively. Any responses that did not appear to clearly fit under a code were discussed and a consensus decision was made. As modifications to the assignment and questions were made during the revision cycles, we used a constant comparative approach to ensure that our codes for each question still captured the breadth of student responses.[37] The coding scheme was modified as needed to include any additional themes (codes) noted in subsequent iterations.

To allow for a quantitative pre-post analysis for a measure of how students' understanding of atomic interactions changed after completing the assignments, responses for each question were assigned a score. Correct pretest questions were given a value of one. The corresponding follow up question was given a value of one if there was one associated question and 0.5 for each question if there were two associated questions. For the claim-evidence-reasoning questions (S1, S3), students were awarded full credit if they provided a correct claim and either correct evidence or reasoning. Using SPSS[38] pretest and follow-up scores were compared using Mixed-design analysis of variance (ANOVA) tests were employed to determine differences in pretest and follow-up scores.

Eye-tracking Study: Participants and Study Design

To characterize the behavior of students' interaction with the simulation and screencast resources, as well as the assignment itself (research question 3), an eye-tracking study was conducted. A total of 16 undergraduate student volunteers participated in the study after covering the relevant prerequisite content in their first-semester general chemistry course. These participants completed the same activities as described in the classroom study; however, they did so in a condensed session lasting approximately 30 minutes. During this session, participants completed both the pretest and follow-up questions using pencil and paper. The screencast/simulation assignment itself was completed while seated at a computer which enabled the capture of eye movements through the Tobii T60 eye-tracking system. This system displayed the assignment and electronic resource (screencast/simulation) on 17-inch computer monitor using a split screen design (Figure 5) and captured participants' eye movements at a rate of 60 Hz. The system was calibrated to each student prior to data collection to ensure accurate measures of eye position for each student. Participants sat approximately 24 inches from the monitor on which the resource/assignment were displayed and had full control of the mouse in order to control the resource and scroll through the assignment as necessary. In order to avoid the need to look away from the screen to record their answers in writing, participants instead gave all answers aloud. These responses were both audio-recorded and recorded in writing by the interviewer to ensure accurate capture. Participants for whom less than 50% of eye positions were captured accurately (according to the Tobii system's recording quality metric[39]) were removed from analysis, resulting in a total of 14 viable participants, 7 participants for each the screencast and simulation treatments.

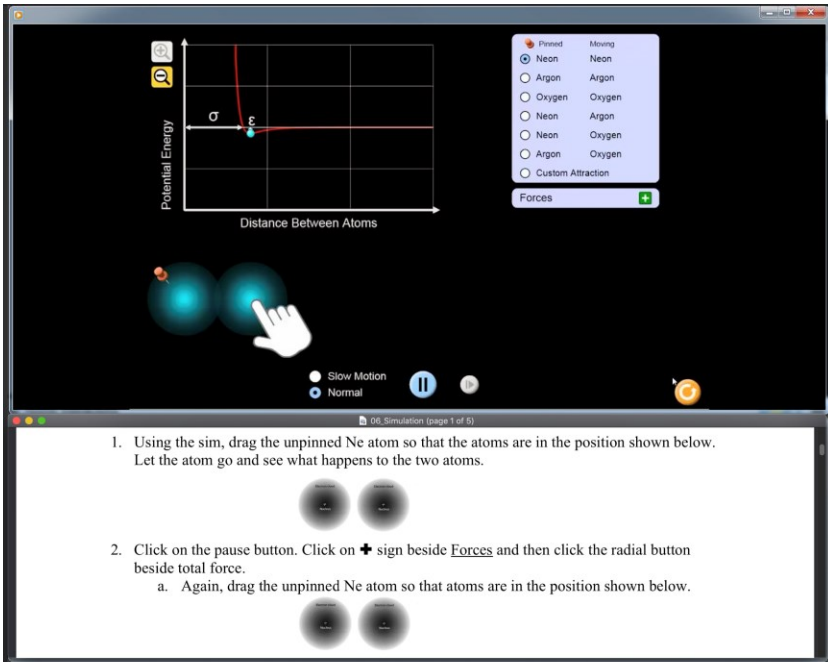


Figure 5. Eye-tracking experimental set-up, showing resource (simulation) at the top of the screen, and assignment at the bottom of the screen. *Simulation image by PhET Interactive Simulations, University of Colorado Boulder, licensed under CC-BY 4.0*

Eye-tracking data were processed using Tobii Studio software in order to identify fixations, with the Tobii Fixation Filter set to a 35-pixel threshold.[39] These fixations were mapped to two areas of interest (AOIs): the electronic resource (top 60% of screen) and assignment (bottom 40% of screen). These two areas of interest were chosen in order to measure how students split attention while working through an assignment while using a simulation/screencast. The split-attention effect has been seen for multi-media materials that convey information from multiple sources along a single modality[40] and results in an increase in cognitive load as students shift attention back and forth to try to integrate multiple sources of information along a single channel. In this case, visual information is being conveyed through on-screen text in the assignment itself, as well as through graphical and particulate images in the simulation/screencast itself. Separating the two regions of visual information into two individual AOIs allows for an investigation of how individuals split their attention between these regions, but also allows us to probe how including information along a second channel in the screencast treatment (audio narration) impacts the manner in which students use the visual resources provided.

The total fixation time within each AOI (in seconds) and the total number of fixations within each AOI were then calculated. In order to compare these metrics among participants, mixed-design ANOVAs were used, with treatment (simulation or screencast) as a between-subjects variable and AOI (resource or assignment) as a within-subjects variable.

RESULTS AND DISCUSSION

Learning Gains

To shed light on research question 1 about how simulations or screencasts can impact student understanding of energy changes at the atomic-molecular level, we examined student learning from the interventions. Student learning was measured based on the difference in scores between the pretest and matched follow-up questions. Since each of the treatment groups began with statistically equivalent pretest scores, a 2 (treatment: screencast, simulation) x 2 (assessment: pretest, follow-up questions) mixed-design ANOVA was used to examine student performance. This test indicated a statistically significant main effect between the two assessments for all students, with an increase in score of 1.39 to 1.83 on a 5-point scale ($F_{1,189}$=19.9, $p<0.001$, η^2_p = 0.10) (Table 4). There was no main effect for treatment or interaction effect between treatment and assessment, implying that there was no difference in performance between students viewing the screencast and those interacting with the simulation. This may suggest that the screencast treatment did not have a significant impact on lowering cognitive load in a way that would allow students to shift resources to processing information to increase understanding and performance over the screencast treatment alone.

In fully considering these results, the pretest score should be viewed as an overestimate of students' incoming understanding, based on the fact that three of the pretest questions were multiple choice.[32,33] A deeper evaluation of the student gains made from pretest to follow-up indicate that they were not evenly split across all the questions and learning objectives (LO): two question pairs saw gains; two remained statistically unchanged; and one showed a decrease. Each question pair was analyzed using an individual mixed-design ANOVA (mean scores for each question pair are shown in Table 4). Results show that question pairs 1 and 2 both demonstrate main effects for assessment (pretest to follow-up), with increases going from 0.06 to 0.44 ($F_{1,206}$=112.5, $p<0.001$, η^2_p = 0.35) and 0.32 to 0.51 respectively ($F_{1,213}$=25.3, $p<0.001$, η^2_p = 0.10) (Table 4). Question 2 also shows a small interaction effect with the treatment ($F_{1,213}$=4.6, p=0.033, η^2_p = 0.021) with the students using the simulation showing greater improvement (improving from 0.32 on the pretest to 0.60 on the follow-up for simulation students, versus 0.44 on the follow-up for screencast students). Questions 1 and 2 both focus on LO 1 (explaining the causal mechanistic reason for attractions), suggesting that many students may be able to productively access and apply prior knowledge regarding opposite charges attracting. With appropriate scaffolding, both the screencast and direct simulation usage can direct student attention on the phenomenon such that many students can productively apply this prior knowledge to provide a scientifically correct explanation that is consistent with this prior understanding.

LO 2 and 3 did not show similar improvements. LO 2 (using PE to explain energy changes associated with bond breaking and forming) was assessed by question pairs 3 and 4. Question pair 4 saw a small, but non-significant, decrease in score for both groups (Table 4). Question pair 3 saw significant decreases in average scores (from 0.31 to 0.19, $F_{1,207}$=8.9, p=0.003, η^2_p = 0.04). A significant main effect for treatment was found for question pair 3, indicating that screencast students performed lower on both the pretest and follow-up (0.26 to 0.15) than did the simulation students (0.37 to 0.24); however, both groups appeared to decrease in performance to approximately the same extent (0.11 points for simulation students and 0.13 for screencast students), indicating that LO 2 was difficult for students regardless of treatment. The results of questions 3 and 4 taken together may be an indication that students' mental models regarding energy changes associated with bond breaking and forming (LO2) is still quite fluid and unstable. This is consistent with the idea that students' prior or intuitive ideas about the energy associated with bonding are not productive in constructing a scientifically correct explanation.[7–10,12,13]

Finally, LO 3 (explaining how strength of interaction and inter-atomic distance is show on a PE graph) was assessed by question pair 5, which also showed no statistically significant change. This indicates that there have been no changes in students' ability to interpret or create energy well diagrams, regardless of treatment. This is perhaps not surprising given students' difficulty interpreting and using graphical representations discussed previously.[16,17]

Table 4. Comparison of pretest and follow-up scores for each assessment question.

	Pretest	Follow up	n	Main effect Pre-Post Comparison	Effect Size (η^2_p)
Total Score	**1.39**	**1.83**	191	$F_{1,189}$=19.9, p<0.001	0.10
Question pair 1	**.06**	**.44**	208	$F_{1,206}$=112.5, p<0.001	0.35
Question pair 2	**.32**	**.51**	215	$F_{1,213}$=25.3, p<0.001	0.10
Question pair 3	**.31**	**.19**	209	$F_{1,207}$=8.9, p=0.003	0.04
Question pair 4	.51	.43	214	--	--
Question pair 5	.18	.24	199	--	--

Bold numbers represent significant differences between the pretest and follow up questions based on a mixed-design ANOVA.

In total, the changes on the individual question pairs are not overly promising. They are a strong reminder that students' understanding of these concepts is still quite fluid and unstable, meaning that the context of the question can result in students accessing different knowledge pieces from which they construct their explanations. Understandably, a single introductory activity, as this was designed to be, does not provide enough experience with the concept for students to reorganize their knowledge into a more coherent and stable model. Ideally, however, the intellectual effort that students expended working on this assignment provide a common starting point for this process upon which to build on in subsequent in-class instruction.

Energy Associated with Bond Breaking Using an Enhanced Screencast

One of the primary goals of this intervention is to help students reorganize their knowledge fragments regarding energy into a more coherent and stable model. However, the lack of pre/post gains on the question pairs targeting LO 2 suggests that this goal was not being met using our initial simulation and screencast treatments. When considering this problem, it was identified that efforts to keep the screencast treatment fully parallel to the simulation treatment meant that we were not taking full advantage of the affordances of the screencast format. In order to answer research question 2 (how can we most effectively use a screencast), the enhanced screencast (described previously) was created to determine if we can leverage the additional benefits of the screencast in order to address LO 2 and improve student learning.

To investigate the impact of the enhanced screencast on LO 2, student performance on question pair 4 was compared using a 2 (treatment: original screencast, enhanced screencast) x 2 (assessment: pretest question 4, follow-up question 4) mixed-design ANOVA. A significant interaction effect was found between treatment and assessment ($F_{1,204}$=5.1, p=0.025, η^2_p = 0.02). Students performed similarly on the pretest whether they were assigned the original (0.52) or enhanced (0.54) screencast assignment. However, on the follow-up assessment, students in the enhanced screencast significantly outperformed students in the original screencast treatment (0.62 for enhanced screencast vs. 0.39 for original screencast). These scores showed that students viewing the enhanced screencast were better able to construct a scientifically accurate explanation. Interestingly across all treatments, most students who made a correct claim were able to supply appropriate evidence from the graph, but of those with correct evidence only 60-70% could provide productive reasoning to complete their explanation. Across all treatments, the students also struggled more with the energy associated with pulling apart atoms than having them come together. These results suggest that a carefully designed screencast with additional relevant examples has the ability to help students reorganize relevant prior knowledge so that they apply it more consistently to different questions that address a challenging learning objective such as those addressed by LO 2.

In addition to question pair 4, a question was added to the follow-up assignment for all students to further probe the impact of the enhanced screencast on student understanding of LO 2. Recognizing that with less stable and coherent mental models the context of a question can activate accessing of different knowledge pieces, we included a biologically oriented question which students have been shown to explain using the idea that bond breaking releases energy[9] to determine whether the treatments were able to help students begin to construct a more coherent understanding of bond energy changes. This question asked students to indicate if bond breaking or forming was related to the release of energy in the specific context of ATP hydrolysis, a context that was previously used in physics education research exploring students understanding of bonding and energy[41,42] (See Supporting Information for specific question). For students experiencing the original screencast, 62% responded that the forming of new bonds releases energy. This is compared to 77% of students using the enhanced screencast, and 70% of students using the simulation alone. Although these groups were shown to be equivalent on their pretest scores, the difference in students answering this question correctly was significant between the enhanced screencast group and the basic screencast group (Odds Ratio = 2.1; 95%CI = 1.1, 3.8) supporting the idea that the enhanced screencast contributed to a more coherent understanding that was transferrable across contexts.

In addition to looking at the percentage of students who correctly answered the ATP hydrolysis question, we can examine how student answers change across the three times that energy changes during bond formation was assessed (pretest, follow-up, and ATP hydrolysis question) to understand how stable their knowledge is across different contexts (Figure 6). 60% of students in the enhanced screencast group who did not provide scientifically correct explanations on the pretest, provided scientifically correct explanations on both the follow-up and ATP questions. This is a statistically significant improvement over the basic screencast, in which only 29% of students who initially provided scientifically incorrect explanations were able to provide scientifically correct explanations for both of the following questions. This suggest that using the screencast to help students explicitly connect energy changes with respect to 2 atoms coming together or being pulled apart with overall energy changes resulting from a chemical reaction can help students reorganize their knowledge and construct a more coherent model that can be applied more consistently across a range of context (e.g. biology).

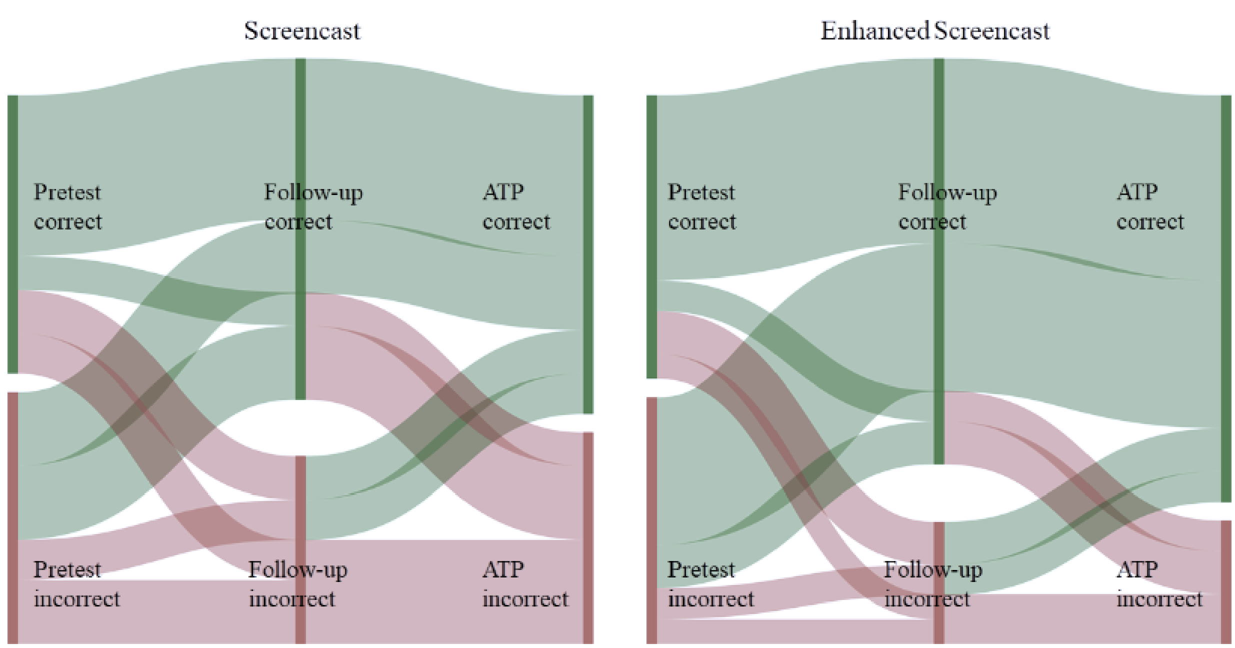


Figure 6. Distribution of students answer about energy of bonds by treatment.

Interestingly, 21% of students using the basic screencast and 12% of students using the enhanced screencast provided a scientifically correct answer on the follow-up question but did not apply this idea in their response on the ATP hydrolysis question. This is despite the questions being essentially identical except for the contexts, thus representing a near transfer task. This suggests that there are still some students who, upon seeing the context of ATP, appear to be accessing their prior understanding about breaking bonds releasing energy rather than reconciling that previous idea with the new information provided in this intervention.

Such an interpretation is consistent with diSessa's concept of "knowledge in pieces".[14] With this framework, the idea that energy is released by breaking ATP molecules apart is representative of a phenomenological primitive (p-prim)—a simple idea from previous experiences that seems straightforward and requires no additional explanation. Seeing the context of ATP in the question could activate the use of this p-prim as the full explanation, without considering the disconnect between this and what they learned in screencast intervention. Instructors must take care, then, to ensure that further instruction strives to challenge inconsistencies in students mental models so as to help them reorganize their knowledge into a more productive and coherent framework that can be consistently applied across contexts.

Eye-tracking Study

To better understand these results through the context of student behavior and to address research question 3, the eye-tracking data were analyzed. Eye movements are a measure of overt visual attention, and the object upon which the eye is focused is also assumed to be the focus of their cognitive efforts.[43] We can therefore assume that students whose eyes are focused on the simulation are thinking about and processing information from the simulation, while those focused on the assignment are thinking about the assignment itself. This use of eye movements as a proxy for mental processing is a commonly used technique that is appropriate for this study, as eye movements have been shown to be highly correlated with think-aloud protocols,[44] demonstrating that both methods reflect similar information about an individual's thought processes. Eye tracking has been chosen specifically to address research question 3 for the quantitative data it provides as well as ease of interpretation over think-aloud protocol analysis.

As previously discussed, eye movements were filtered to identify fixations, moments in time when the eye is relatively still and the majority of mental processing is assumed to take place.[45] Both the number of fixations an individual makes and the total amount of time spent fixating can be used to make inferences about mental processing. For example, an individual may make a large number of very short fixations when they are searching a scene for a particular object, or they may make a low number of very long fixations if they are intensely scrutinizing a single object. For this reason, both the number of fixations and total fixation duration in each of the AOIs (electronic resource and assignment) were measured. As with previous studies,[29,46] however, these metrics were shown to be highly correlated ($r=0.708$, two-tailed $p=0.005$); for this reason, only fixation duration was analyzed for the remainder of this study.

In order to investigate how students allocated attention between the electronic resource and the assignment questions, a mixed-design ANOVA was used. Full results of the ANOVA are given in Table 5. A significant interaction was found between treatment (simulation vs screencast) and AOI (resource vs assignment) for total fixation duration ($F_{1,12}=5.185$, $p=0.042$, $\eta^2_p=0.302$). In the presence of a significant interaction effect, other main effects were not probed further. As the data in Table 6 show, all students spend more time viewing the assignment itself than they do viewing the electronic resource, regardless of treatment. However, we can see that students using the simulation spend a greater amount of time on the assignment than do the screencast students. These results suggest two things. First, it is possible that this simple simulation, which presents limited visual information, has minimal extraneous cognitive load. This suggests that it is relatively easy to understand by students and they do not need to spend a large amount of time to decode its meaning. This is consistent with the relatively low amount of time spent fixating on the simulation or screencast and larger amount of time to read and understand the assignment questions. Second, the fact that simulation students spend more time reading and responding to the assignment questions suggests that the screencast lowers student cognitive load, perhaps through directing attention to relevant features, allowing the questions to be more easily understood in context. These results taken together suggest that even for less cognitively demanding simulations, screencasts may provide students with a distinct advantage in sense-making of both content and instructor questions.

Table 5. ANOVA Results for Fixations on Assignment vs Electronic Resource

Effect	Wilks' Lambda F1,12	Significance	Partial Eta Squared
Main: Treatment	1.083	0.319	--
Main: AOI	42.437	0.000	0.780
Interaction: Treatment x AOI	5.185	0.042	0.302

Table 6. Mean fixation durations by treatment for assignment (guiding questions) and resource.

Treatment	Fixation Duration, Mean [SD] (sec)	
	Assignment	Resource
Screencast (N=7)	434 [76]	333 [54]
Simulation (N=7)	535 [151]	325 [62]
Total	485 [126]	329 [56]

However, the concern still remains that students who view the screencast have not had direct interaction with the simulation. Lacking this interaction has the potential to decrease student learning, but also may hamper students' ability to use the simulation themselves when necessary, increasing the extraneous load when these students begin working with the simulation. All students were instructed to use the simulation to answer the "Going Further" question in the assignment, whether they had been using it all along (simulation students), or whether they had previously only watched someone else manipulate the simulation (screencast students). A mixed-design ANOVA on fixation duration for students responding to these questions shows only a main effect for AOI ($F_{1,12}$=28.778, $p < 0.001$, η^2_p =0.706), with no interaction effect for treatment (Table 7). This suggests that students demonstrate the same pattern of behavior as they do during the assignment itself, spending significantly more time reading and responding to the assignment as opposed to viewing the resource (Table 8). The lack of significant interaction effect, however, shows that both screencast and simulation students are using the resource for the same amount of time; screencast students have not been hampered in their ability to use the simulation. Even though this is their first opportunity to control the simulation directly, they do not require any more time to use or understand the simulation than do the students who had been using the simulation for the entire assignment, suggesting cognitive load has not been negatively impacted by introducing this new tool. These results are promising and suggest that the screencast can be an effective introduction not only to a chemistry concept, but also to the use of the simulation itself. Instructors who want students to have the experience of manipulating the simulation on their own need not worry that the screencast will interfere with students' ability to make sense of the simulation or slow down their progress in any way.

Table 7: ANOVA Results for Fixations on Going Further vs Electronic Resource

Effect	Wilks' Lambda F1,12	Significance	Partial Eta Squared
Main: Treatment	0.094	0.765	--
Main: AOI	28.778	0.000	0.706
Interaction: Treatment x AOI	0.686	0.424	--

Table 8. Mean fixation durations by treatment for Going Further Questions.

Treatment	Fixation Duration, Mean [SD] (sec)	
	Assignment	Resource
Screencast (N=7)	398 [111]	221 [75]
Simulation (N=7)	417 [161]	175 [80]
Total	407 [133]	198 [79]

LIMITATIONS

This study was conducted at two different institutions and provided consistent results across both settings with many different instructors throughout the different iterations of the material development. This suggests that the results are likely to be similar in other settings. As this activity was completed outside of the classroom, we anticipate that the classroom environment may only have minimal impact. However, both courses that participated in this study have a focus on helping students develop conceptual understanding of chemical phenomena. It is possible that the results may vary in a setting where a higher emphasis were placed on mathematical calculations. Yet given that this is a first semester course where many students are developing their ability to provide meaningful explanations, this may be surprising.

It should also be noted that this assignment is an introduction to the topic of potential energy and is meant to be a foundational experience upon which the instructor can build during subsequent instructions. The materials do not fully address why some atoms form covalent bonding and others only form intermolecular forces. Further, they focus solely on potential energy as it relates to attractive and repulsive forces between atoms and instructors would be expected to provide additional support for students to meet the learning expectations for their classes.

In the enhanced screencast, our added description of the energy changes associate with the combustion of methane shows that all the bonds are broken prior to being reformed to make products. We recognize that this is not the actual mechanistic pathway by which this reaction happens, and that this representation has the potential to give students the idea that reactions proceed by reactants completely falling apart and then reforming. As instructors we are aware that all of the models that we use have limitations and it is incumbent upon us to make our students aware of them too.

CONCLUSIONS AND IMPLICATIONS FOR TEACHING

Results from this study highlight the challenging nature of helping students develop a coherent and stable understanding the energy changes associated with atomic interactions for students. Although all students, regardless of treatment, showed an average increase from pretest to follow-up after interacting with the guided simulation or screencast assignments, their overall scores were still less than 40% (1.83/5) on the follow-up questions. The gains were concentrated on questions associated with LO 1, the mechanistic basis for attractive forces. The same success was not present on LO 2 and 3 which address concepts that students are more likely to have more inconsistent and unstable ideas (the energy associated with bonds) or prior difficulty (graphical representations). This reaffirms that difficult concepts cannot be readily mastered with a single intervention but remind us that out-of-class interventions may serve as a strong foundation for classroom instruction. Introducing a new topic through simulation or screencast assignments gives students a common experience from which the classroom teacher can build, and allows them to make observations and collect data that can be used to help the students align their multiple understandings of energy into a single, unified, conceptual understanding of energy in the classroom with direct instructor support.

In comparing the effectiveness of stand-alone simulations versus an introductory, instructor-led screencast, few differences were found in terms of student performance. This stands in contrast to previous studies employing other simulations that have shown significant differences in both performance and behavior between screencast and simulation treatments,[28,29] as well as the anticipated outcome that the screencast may lower cognitive load an allow for improved performance. Eye-tracking results suggest that this may be due to the simplicity of the simulation itself. Where previously studied simulations incorporated multiple screens[28] or multiple particulate and graphical representations on a single screen,[29] the Atomic Interactions simulation uses a single screen, and showed only one graph and the interaction of only two atoms at a time. This simpler visual stimulus may have presented students with lower extraneous load than previously studied models. Students are seen to fixate on the resource for approximately the same amount of time whether they are viewing the screencast or interacting with the simulation, demonstrating that extra time may not have been needed to decode and understand this simple simulation. However, simulation students did spend more time viewing the questions themselves, possibly indicating that without the benefit of the screencast to explain the context of the questions, students may require more time and cognitive effort to process and understand the assignment. Therefore, although the screencast may not offer a significant advantage in terms of performance (pretest to follow-up), it may still be useful to incorporate the screencast as an introduction to the simulation itself, lowering cognitive demand and making the assignment feel easier for students to complete.

Finally, in an effort to compare the effectiveness of screencasts and simulations directly, care was taken to make these treatments as parallel as possible. This meant ignoring some of the potential benefits of screencasts, such as including additional information, graphical representations, etc. An enhanced screencast allowed us to investigate some of these advantages by including an additional example extending the simple two-atom systems shown in the simulation to the more complex combustion of methane. Students who viewed this enhanced screencast were able to more consistently provide scientifically correct responses to questions about the energy associated with bond making and breaking, suggesting that extending screencasts to incorporate additional information may be a worthwhile endeavor in supporting the use of simulations outside of the classroom to support student learning of difficult chemistry concepts.

Overall, classroom teachers may benefit from using either a screencast or simulation as an introduction to a complex topic such as atomic interactions. The screencast may offer some benefits in terms of making this introduction feel easier for students, particularly if instructors add additional information to the screencast to extend its applications to more complex topics.

SUPPORTING MATERIALS

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.XXXXXXX.

Pretest Questions

Assignments

Coding Scheme

AUTHOR INFORMATION

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