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From Abstract to Manipulatable: The Hybridization Explorer, A Digital Interactive for Studying Orbitals

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ABSTRACT: As digital educational media use becomes more widespread, an opportunity exists to develop new methods to present abstract ideas to provide a more meaningful learning experience. Drawing from psychology and dynamic visualization research, new interactive tools can be thoughtfully designed but it is also necessary to establish how these media are used and to study the effects the new interactive tools have on concept understanding. In this technology report, we present the Hybridization Explorer, a web-based interactive learning tool for manipulating and experimenting with hybridization concepts. The explorer has three modes of use to explore both the combination of atomic orbitals, and the visual representation of both atomic and hybrid orbitals and corresponding bond formation. Case studies from an undergraduate- and graduate-level demonstration of the explorer are described. Finally, self-reported student confidence levels on solving hybridization questions both before and after use of the explorer are analyzed and discussed.

KEYWORDS: *General Public, First-Year Undergraduate/General, Second-Year Undergraduate, Curriculum, Demonstrations, Hands-On Learning/Manipulatives, Internet/Web-Based Learning, Covalent Bonding, Valence Bond Theory, VSEPR Theory*

Hybridization theory is abstract and difficult for students to grasp and understand. When students enter a chemistry course, they do not bring in any preconceived beliefs regarding hybridization as this concept is not experienced in everyday life.[1] Yet the literature reports that students develop numerous alternative conceptions regarding hybridization.[1−4] Problematically, this means that misconceptions develop as a result of their chemistry studies including, but not limited to, textbook reading, lecture, homework, studying with peers, and online searches. While this notion is disconcerting, Taber offers the encouraging perspective that (ref 1, p 130) "this should not be taken to mean that 'we only have ourselves to blame' (after all: chemistry is complex, teaching is difficult, and pedagogy is poorly developed), but rather that to some extent we have the power to make things better for learners."

The first step in improving the pedagogy is to identify where and why students are struggling with hybridization.[5] Nakiboglu has summarized many of the identified alternative conceptions regarding orbitals and hybridization.[3] A commonality in these conceptions is the attempt of students to connect new information about orbitals to prior knowledge that is irrelevant including electron shells, the octet rule, electron configurations, and an idea that electrons orbit like planets around the sun. What also stands out is students' lack of ability to visualize the shape and directionality of both atomic and hybrid orbitals. In fact, several researchers have recommended that pedagogy focus on improving students' ability to visualize atomic and hybridized orbitals to enable conceptual understanding of hybridization theory.[2−4,6,7] To meet this need, physical manipulatives, such as balloons and 3D-printed orbitals, can be used during lectures as a concrete representation.[8,9] Digital models of hybrid orbitals, while less common than the more accurate molecular orbital, are available via CheMagic,[10] via ChemTube3D,[11] or by the open-source Java viewer for chemical structures, Jmol.[12,13] We observed that a limitation of these methods is the low availability of physical models for students to manipulate and explore on their own, existing digital models feel intimidating and are not straightforward to use, and it is not practical to use these tools for assessment of student understanding of orbital representations.

Currently the most readily available orbital representations are static two-dimensional images commonly provided in textbooks.[14−21] Basic research from psychology has found that mental representations of objects are largely viewpoint

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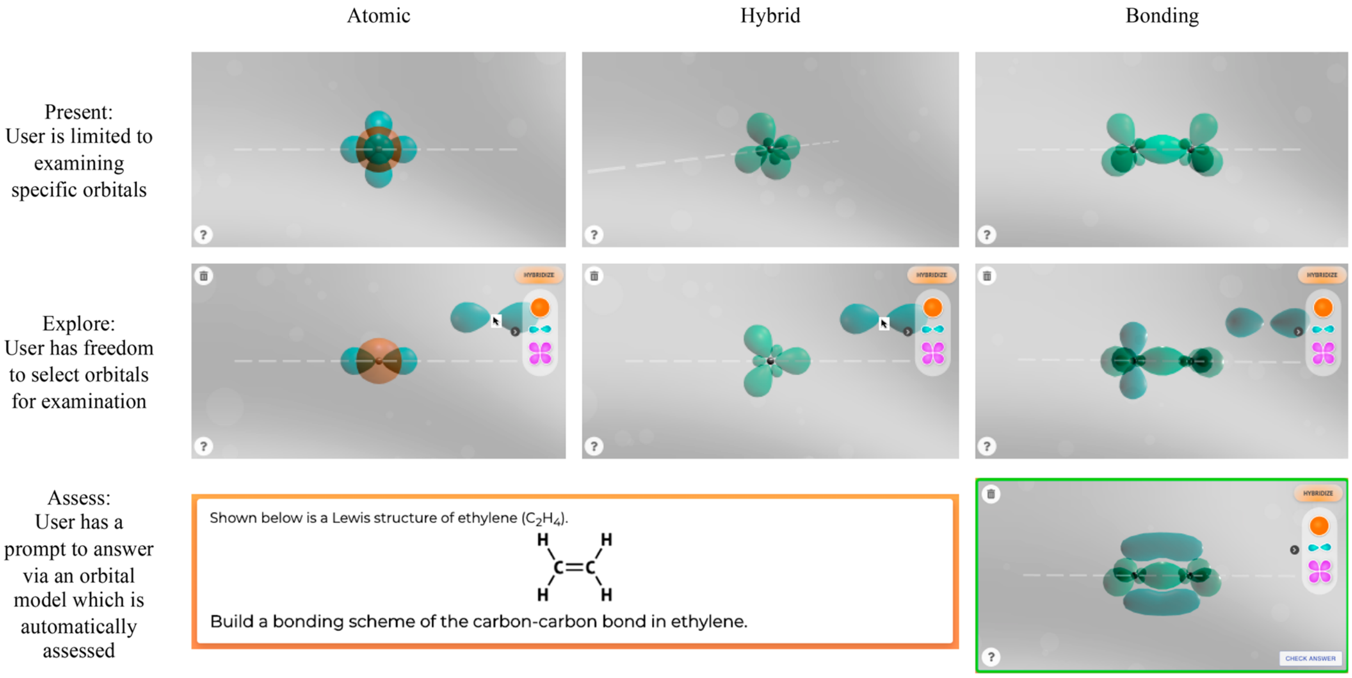

Figure 1. Samples of the representations generated in the Hybridization Explorer of atomic orbitals, hybrid orbitals, and bonding, in each of the three modes, Present, Explore, and Assess. These screen shots are "in action". For example, the axis is rotated for present of the sp^3 hybrid orbitals and the p orbital is being dragged by the user in the explore and assess screen shots. Screen shots courtesy of Alchemie Solutions, Inc.

dependent and stored as an individual view.[22−24] Put into context, this means that students do not naturally take static two-dimensional images of orbitals and rotate them to generate a three-dimensional model. As a result, it is difficult to apply a mental image of orbitals to different atoms or molecules not previously presented to them. Another challenge that static images present is that a single viewpoint is typically not sufficient for grasping spatial relationships, and sometimes relevant parts are occluded.[24] In general, the flexibility of one's mental representations can be improved by studying multiple viewpoints or continuous movement around an object, as is now possible with digital models.

On the basis of students' struggles to understand hybridization theory, the imminent transition of textbooks to a digital format,[25] the prevalent use of digital homework systems, widespread availability of computers, and advances in technology, we saw the opportunity and need to generate a digital interactive for studying atomic and hybrid orbitals. To fill this void, we designed and constructed the "Hybridization Explorer" with the objective of creating a tool to help students visualize and feel the three-dimensional nature of orbitals in an intuitive framework.

In this technology report, we describe the key features and content of the Hybridization Explorer. Also included are self-reported confidence levels of students in solving hybridization-type questions before and after using the explorer, student feedback regarding the explorer, and two case studies detailing the use of the explorer in an undergraduate- and a graduate-level course.

■ HYBRIDIZATION EXPLORER

Design of the Interactive

Inspired by Bruner's theory of constructivism,[26] we believe that complex topics can be taught to anyone at any age when the basic ideas are presented in an intuitive or experiential way. Confounding the study of hybridization, the terms used to describe the model are difficult to understand until a conceptual knowledge is developed.[1] Many of these terms carry spatial information, such as the tetrahedral geometry of sp^3 hybrid orbitals, that is not intuitive to picture mentally nor easy to draw. Research has shown that when invisible chemical phenomena are made visible through the use of visualization tools, such as animations and simulations, student learning outcomes improve.[27] These tools are more effective when incorporated with inquiry activities, thereby promoting interactivity.[27] We also identified the need for a manipulative that can be experienced by the students. It has been found that it is not enough for students to just observe the use of a manipulative; to improve representational competence students must interact with the models themselves.[28] Therefore, to enable a more experiential and therefore accessible pedagogy, we chose to create an interactive explorer of atomic and hybrid orbitals. We propose that an interactive is superior to an animation as the interactive allows for student engagement and integration into active learning teaching practices.

The Hybridization Explorer is a web-based interactive that can be accessed through any web browser.[29] Our learning objective in developing the explorer was to create a visualization tool to help students see and feel the three-dimensional nature of orbitals. To meet this objective, the explorer allows users to rotate and study a three-dimensional representation of atomic orbitals, hybrid orbitals, orbitals of a single atom, or orbitals on two neighboring atoms and the resultant σ and π bonds. This explorer is not intended to serve as a standalone pedagogical tool but instead designed to be readily incorporated as a supplement to existing pedagogies in digital textbooks, Open Educational Resources (OERs), and homework systems.

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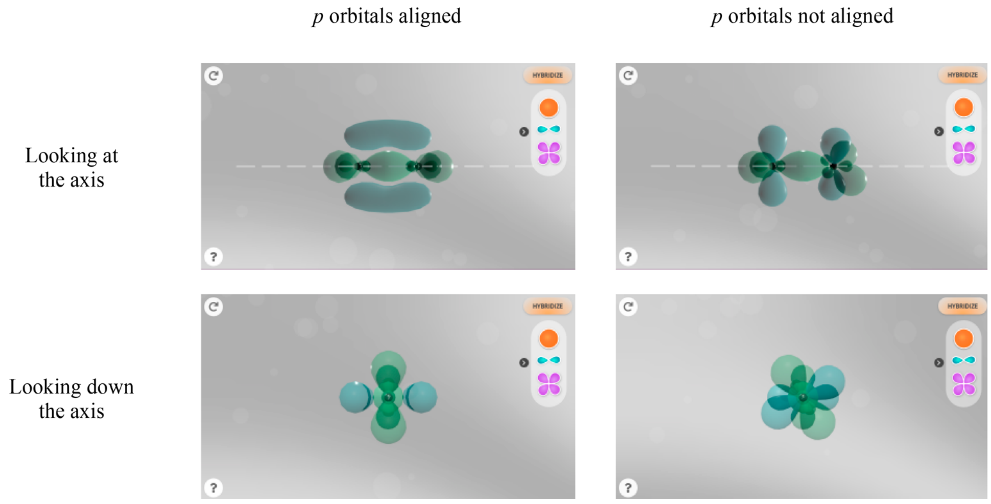

Figure 2. Sample visuals in the explorer for when the p orbitals are aligned for π bond formation and after rotation of an atom so that the p orbitals are not aligned and no π bond is present. Camera angles looking at the axis (default) and looking down the axis, to more clearly see if the p orbitals are aligned, make for a more complete representation. Screen shots courtesy of Alchemie Solutions, Inc.

To facilitate curricular design, three modes of the explorer were developed: Present, Explore, and Assess (PEA) (Figure 1). In present mode, the user cannot add or subtract atomic orbitals but only rotate the orbitals present to gain viewpoints from multiple angles. Additionally, if all of the orbitals present are atomic orbitals, users can click hybridize to view the resulting hybrid orbitals. In explore mode, a user can drag and drop atomic orbitals onto a black dot and explore the geometries. Users can also click hybridize to generate the hybrid orbitals and add any unhybridized atomic orbitals that are left over to generate a complete orbital model. If two atoms are present, then a user can explore the bonding between those atoms by clicking and dragging on one black dot to rotate just that atom. If a π bond is present, then the π bond will break when the p orbitals are not aligned and re-form when rotated back into alignment (Figure 2).[30] Prompts that can be answered via orbital diagrams can make use of assessment capabilities of the explorer. In assess mode, the orbital representation built by the user is automatically graded against a goal configuration.

■ USE STUDIES

To date, the Hybridization Explorer has been incorporated into a general chemistry lecture, an active learning physical organic chemistry lecture, and as part of a hybridization review web page in a research study. Detailed below are the experiences and observations of the instructors of these courses and the researchers, who are also coauthors. Also reported is the change in students' self-reported confidence levels in answering hybridization assessment questions before and after using the explorer.

Limitations

Since the Hybridization Explorer is not a stand-alone tool, how it is implemented will affect its effectiveness. In these reports, either the instructor demonstrated the explorer and gave verbal explanations or students were given specific tasks and questions to answer while using the explorer. Therefore, the goal of this discussion is to highlight initial impressions and observations of students' experiences with the interactive orbital models.

General Chemistry Class Demonstration

In an effort to probe student reactions to the Hybridization Explorer tool, the interactive was demonstrated in front of a class of 30 students. While covering hybridization and bonding, the normal lecture material was presented and then shown using the Hybridization Explorer tool. Lecture began with sp^3 hybridization showing the usual static images from the textbook; these textbook figures generally illustrate a collection of atomic orbitals arranged to mimic the formation of the requisite sp^3 hybrid orbitals. This is capped with a summary figure of the four equivalent sp^3 hybrid orbitals. This discussion of sp^3 hybrid orbitals was immediately followed up with coverage of sp and sp^2 hybrid orbitals with the same general format of using static figures. A summary of these types of hybrid orbitals was then presented in a table format.

Next, an analogy of hybrid orbital formation with that of baking cookies was made. When baking cookies, a recipe with prescribed amounts of ingredients is used, and after baking, the resulting cookies are a hybrid of the initial ingredients. Hybrid orbitals are formed by using a "recipe" of atomic orbital ingredients. From past experience, students seem to remember the analogy but fail to understand what the process of hybridization really is because cookies are a tangible reference point while atomic orbitals are not. It is here that a demonstration of the Hybridization Explorer tool was given as a way to visualize the "baking" of atomic orbitals.

The demonstration began by referring back to sp^3 hybrid orbitals and how, from earlier in the lecture, they know that it requires one s atomic orbital and three p atomic orbitals. The Hybridization Explorer allowed for spatial arrangement of the atomic orbitals to show the geometric constraints of trying to employ atomic orbitals in bonding. Then with a simple press of a button, these atomic orbitals hybridized into the resulting sp^3 hybrid orbitals. One of the more significant conceptual disconnects students face with orbital hybridization is the geometric arrangement of atomic orbitals relative to that of hybrid orbitals. With this tool, it was easy to rotate completely around to fully understand how mutually perpendicular p atomic orbitals coupled with a spherical s atomic orbital can give rise to the tetrahedral arrangement of the sp^3 hybrids.

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This demonstration was then repeated with the sp and sp^2 hybrid orbital cases. Again, the Hybridization Explorer allowed us to investigate the geometric constructs of hybrid orbitals with the added insight now of visualizing what it means to have unhybridized atomic orbitals in conjunction with hybrid orbitals. The student reaction to this tool overall was very positive especially regarding seeing the process of hybridization occur in real time. After this lecture period was over, several students commented how they wished they could play around with the tool themselves.

Physical Organic Chemistry In-Class Activity

In this physical organic chemistry class, there was a mixture of advanced undergraduate and graduate students and active learning techniques were used during lecture. To start the semester, a review of key concepts, such a bonding, were covered. The Hybridization Explorer, while designed for lower level courses, was used for reviewing hybridization theory because students could readily build, view, and refer to orbital models, and this activity helped to facilitate discussions. During lecture, students were given access to a web page with the explore mode for a single atom and a two-atom system. Students worked in groups to build specific models and answer prompts from basic ideas such as "how does each model show the 'conservation' of orbitals upon hybridization?" to more advanced ones like "rank the hybrid orbitals in terms of their ability to shield the nucleus." Finally, a whole class discussion, led by the instructor, was used to solidify understanding.

During the class period, students were highly engaged and able to use the Hybridization Explorer with little guidance. While the prompts focused on sp^3, sp^2, and sp hybrid orbitals, numerous students were observed to be exploring sp^3d and sp^3d^2 out of curiosity. After class, a survey was sent to students asking if they thought the Hybridization Explorer was **not** particularly helpful. Out of 30 students, 21 responded and 70% of them strongly or somewhat disagreed with the statement. Students were also prompted to explain their choice. Those who agreed with the statement said they felt like they already had a strong understanding of hybridization theory, so the explorer did not help them. Students who disagreed with the statement frequently stated that the explorer was most helpful with visualization of the orbitals and they felt like they got a "hands-on" approach to reviewing orbitals that was "fun and immersive". Across the board, students commented how it would have been helpful to use the tool in an earlier chemistry course. Overall, the explorer helped make it so that all students had similar mental visualization of orbitals which was necessary for the more advanced understandings that were developed throughout the remainder of the semester.

Confidence Levels Changes

A key objective in developing the explorer was the hypothesis that conceptual understanding of hybridization theory is hindered by lack of models to give complete visualizations of the orbitals. Upon completion of the first version of the Hybridization Explorer, a phenomenography study, deemed exempt from IRB review by Sterling IRB (IRB ID No. 7603-SWegwerth), was conducted to investigate students' experiences using the explorer (see the Supporting Information for additional details). Think-aloud interviews were held with 31 undergraduate students who had prior hybridization theory instruction. During the interview participants answered common hybridization assessment questions (Supporting Information) regarding the molecule in Figure 3, used the explorer as part of a hybridization review web page, and filled out a blank copy of the questionnaire. Both before and after using the explorer, participants were asked to self-rank their confidence level (guessing, not confident, confident, very confident) after answering each question. Literature reports students are more confident in answering algorithmic-based questions, so included were questions that varied from an algorithmic to a conceptual basis.[31,32] One goal of the explorer is to empower students to be confident in applying conceptual knowledge to answer hybridization questions, which can even assist in answering algorithmic-based questions. Therefore, rather than survey students about if they like the explorer, a comparison of confidence levels before and after using the explorer was used as a gauge for successfulness.

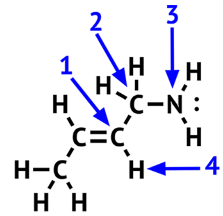

Figure 3. Lewis structure used on the questionnaire.

The changes in confidence levels were analyzed for each question individually using Sankey diagrams, shown in Figure 4–6. Because the type of question may impact confidence levels, the Sankey diagrams will be discussed in order of

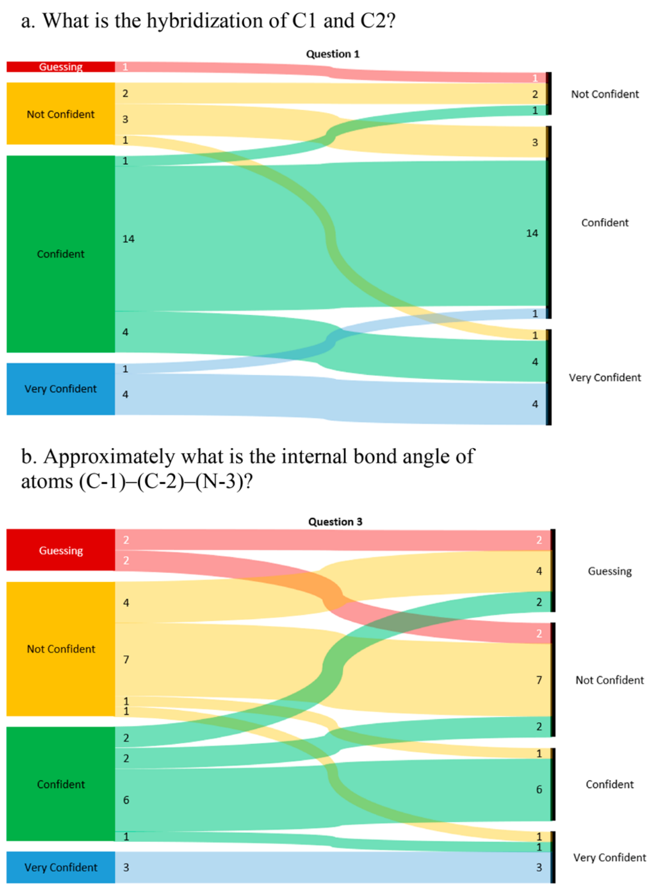

Figure 4. Sankey diagrams showing the change in participants' self-reported confidence levels before and after using the explorer for (a) question 1 and (b) question 3.

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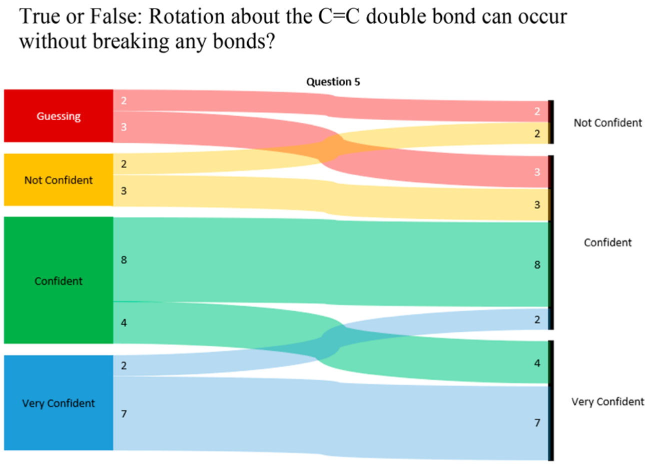

Figure 5. Sankey diagram showing the change in participants' self-reported confidence levels before and after using the explorer for question 5.

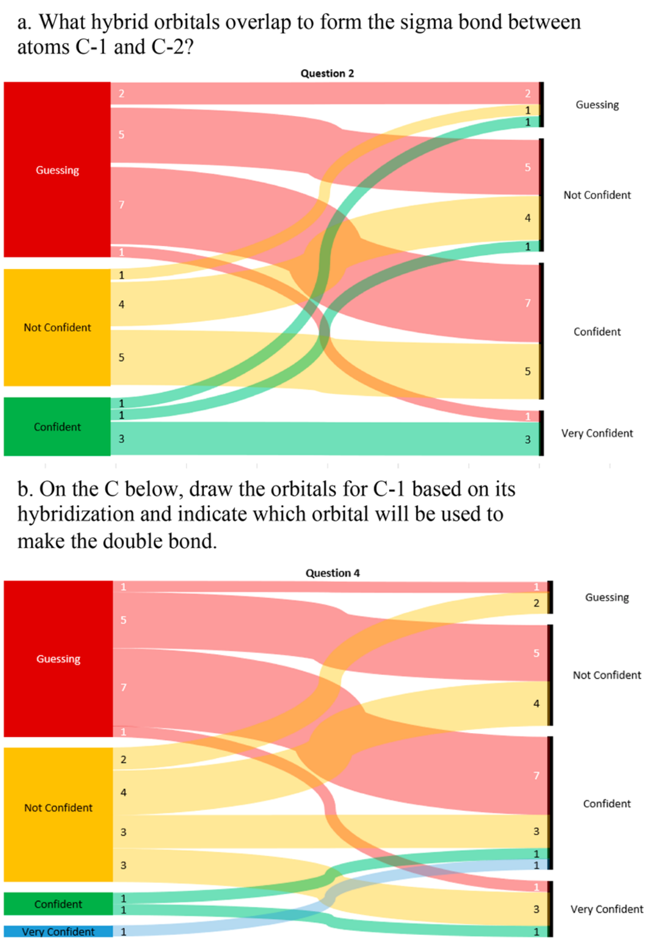

Figure 6. Sankey diagrams showing the change in participants' self-reported confidence levels before and after using the explorer for (a) question 2 and (b) question 4.

increasing conceptual basis. The strategies used, and the knowledge pieces gained, lost, or connected while using the explorer, are important parts of the study and will be discussed elsewhere.

Beginning with the algorithmic, question 1 (Figure 4a), identifying the hybridization of an atom, participants answered the most confidently both before and after using the explorer. Most notably, after using the explorer, no one guessed and 87% of participants were confident or very confident in their answer. For question 3 (Figure 4b), identifying the bond angles of an sp^3 carbon, there was a notable decrease in confidence levels. This correlates to the inability of many participants to identify the angle between the orbitals of a sp^3 hybridized atom in the explorer. The decrease in confidence further signals the need to add additional scaffolding, such as a toggle to show the outline of a tetrahedral or axis through each orbital, to improve the visualization of bond angles in the explorer.

Question 5, probing about the ability to rotate a π bond, could be answered by simple fact recall but the basis for the answer relies on an understanding of p orbital overlap. While a majority of participants were confident in their answer, both before and after using the explorer (Figure 5), after using the explorer, no participants reported guessing and only 13% were not confident. While using the explorer, participants were asked to rotate an atom of a double bond, and most interpreted the disappearance of the π bond as the breaking of the bond. That observation, along with the increase in confidence levels, suggests the visuals for π bonding are effective.

Questions 2 and 4 were the most challenging for participants as there was no algorithm that could be applied. Prior to using the explorer, nearly 50% of participants report guessing for each question (Figure 6). After using the explorer, these questions had the largest increase in confidence, by far, with many students even making the jump from guessing to confident. The commonality between these questions and question 5 is the foundation for answering relies on a visualization of orbitals. Therefore, these increases in self-reported confidence level are a strong indicator that students feel capable of using the models presented in the explorer to develop answers.

FUTURE WORK

Future work on the explorer includes investigating how best to portray bond angles and identifying and correcting misconceptions that develop as a result of using the explorer. Work is also being done to incorporate the interactive into curricular materials including digital textbooks and homework systems. During this process, investigation of best practices for implementation and long-term impact studies will be of great value. Also pressing is the need to make the explorer accessible to all, including those who are visually impaired. This effort will involve a combination of physical manipulatives with audio-based augmented reality to provide guidance for independent exploration.

Undoubtedly, the question of how to help students develop a better conceptual understanding of hybridization is multifaceted. As a step toward this goal, the Hybridization Explorer has been designed to make the abstract, in this case orbitals, manipulatable. From the use studies, clearly students are receptive of the visualizations presented in the explorer and find them helpful. While these studies focused on use of the explorer as a learning tool, the explorer can also be used for assessment. In fact, it is anticipated that the explorer will lower the barrier to asking conceptually based questions that involve invoking orbital models.

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■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00847.

Confidence-level study methods and questionnaire (PDF)

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Notes

The authors declare the following competing financial interest(s): The Hybridization Explorer is a product of Alchemie Solutions, Inc., and authors Sarah Wegwerth, Julia Winter, Gianna Manchester, and Joseph Engalan have received compensation for work performed as employees of Alchemie. The authors Jason Overby and Christopher Douglas declare no competing financial interests.
Demonstration information of the Hybridization Explorer can be accessed at https://alchemie-interactives.web.app/demo.

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