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How Do Inorganic Students Represent Molecular Orbitals? A Multi-Institutional Study from the Foundation-Level Inorganic Chemistry Course

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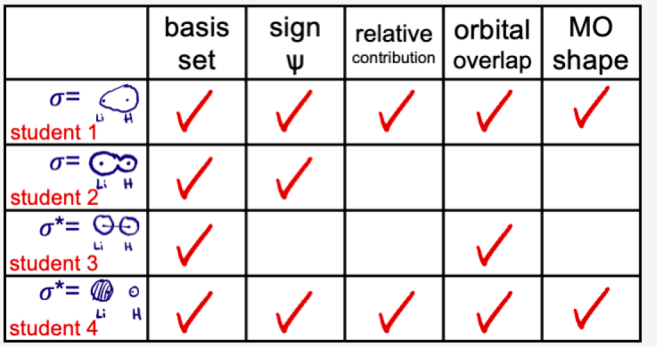
ABSTRACT: This investigation of student and instructor representations of molecular orbitals (MOs) uses the knowledge from a community of practice to build collective pedagogical content knowledge of student understanding of molecular orbital representations in the foundation-level inorganic chemistry course. Participants were asked to sketch the bonding and antibonding MOs of a lithium hydride molecule. The student-generated images of MOs were analyzed and characterized according to five criteria: the atomic orbitals chosen, the sign of the wavefunction, the relative contribution of the atomic orbitals to the molecular orbitals, the overlap of atomic orbitals, and the shape of the MOs. While most students correctly chose a basis set and accurately represented the sign of the wavefunction for the MOs, they were less successful at sketching the relative contribution of the atomic orbitals to the molecular orbitals, the overlap of atomic orbitals, and the shape of the MOs. Students have an incomplete understanding of the information encoded in MO sketches and may not attribute meaning to these pictures in the same way that instructors may. These results suggest that instructors need to help students develop representational competence in order to achieve a more expert-like understanding of MO representations and to connect these depictions to the properties of molecules.



KEYWORDS: *Upper-Division Undergraduate, Inorganic Chemistry, Misconceptions/Discrepant Events, MO Theory, Covalent Bonding*

INTRODUCTION

Bonding is a core concept repeatedly addressed throughout the undergraduate chemistry curriculum.[1] To fully demonstrate an understanding of bonding, learners must integrate their conceptual knowledge and representational competence while choosing among an array of bonding models to predict and explain a system. The complexity of bonding models increases as learners progress through the curriculum;[1] students typically advance from Lewis and valence bond models in general and organic chemistry toward more quantum mechanical, molecular orbital (MO) theory models in upper-level courses such as physical chemistry. In inorganic chemistry, which may require prior coursework in physical chemistry, students are expected to select and apply all of these bonding models. MO theory is central to foundation-level inorganic chemistry courses; >95% of faculty cover this topic in their courses.[2] A learning goal that is common to most inorganic chemistry courses is constructing MO diagrams for diatomic molecules and using them to describe properties (e.g., bond length, bond strength, and magnetism). Furthermore, learners must be able to draw and interpret molecular orbitals and their corresponding energy diagrams to demonstrate an understanding of bonding and associated concepts.

Evidence-based teaching strategies have been shown to positively impact learning and improve learning outcomes in undergraduate science, technology, engineering, and math (STEM) courses.[3−6] To implement such strategies, instructors need to combine their understanding of the content (i.e., content knowledge) with their understanding of teaching (i.e., pedagogical knowledge) to develop their pedagogical content knowledge (PCK). PCK is an instructor's knowledge of student understanding and instructional strategies specific to a topic. PCK has been shown to help instructors promote deeper learning by their students.[7−10]

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Critical elements of PCK are developing familiarity with what students know about a topic; the common difficulties encountered when integrating new ideas into existing knowledge; and the naive ideas, alternative conceptions, or variations in student thinking. Multiple reviews have examined student ideas about chemical bonding.[11−14] Most of the published work has focused on secondary school and general chemistry courses[15−17] rather than upper-level courses that promote a more sophisticated understanding about bonding. While individual instructors may have ideas about what students know about MO theory derived from their teaching experience, this knowledge is typically not shared and is inaccessible to other instructors. By uncovering these ideas through our work that leverages a community of practice such as the Interactive Online Network of Inorganic Chemists (IONiC),[18] we hope to accelerate the process of building shared PCK about students' conceptual understanding of bonding for the inorganic chemistry education community.

In this article, we describe how members of the IONiC community collaboratively developed insight into what students know about MO theory. Specifically, we report how inorganic chemistry learners and instructors represent MOs. Nine faculty members at different institutions teaching a one-semester, foundation-level inorganic chemistry course assigned an open-ended conceptual assessment to their classes ($N = 248$ students). The assessment asked respondents to sketch MOs for lithium hydride (LiH) when given an MO diagram and sketches of MOs of H_2 for reference. They were then asked to explain what information is provided in the MO sketches. The representations constructed by students and instructors contribute to the body of PCK on teaching MO theory. Our analysis of the MO drawings provides implications for improving teaching and learning in the context of foundation-level inorganic chemistry courses. In particular, our work suggests ways to promote representational competence when learning about bonding and highlights important elements of MO sketches.

PEDAGOGICAL CONTENT KNOWLEDGE AND CHEMISTRY INSTRUCTION

In a discipline, the awareness of student alternative conceptions and developing strategies to address noncanonical conceptions comprise part of an instructor's pedagogical content knowledge (PCK). PCK, initially described by Shulman, is knowledge of effective strategies for teaching specific disciplinary content.[19] PCK intersects content knowledge and pedagogical knowledge. To be an effective instructor, one must be more than a content expert who knows something about teaching; instead, one must know "the most useful ways of representing and formulating the subject" for others.[19] An instructor with highly developed PCK takes their topic-specific content knowledge and uses students' prior knowledge and common difficulties to select examples and design instructional strategies to support learning. This endeavor can be supported or hindered by course materials such as textbooks (vide infra).

Over time, PCK was elaborated by others in several ways. Magnusson, Krajcik, and Borko brought many ideas together into a framework called "the refined consensus model of PCK".[20] This framework describes five types of knowledge that make up an individual's PCK: assessment knowledge, content knowledge, curricular knowledge, knowledge of students, and pedagogical knowledge. The model also describes three PCK levels: collective PCK or the cumulative knowledge of the community, personal PCK or the knowledge held by individuals, and enacted PCK or the knowledge used in teaching. Rodriguez and Towns have encouraged chemistry education researchers to use this framework when describing the relevance or implications of their findings for practitioners.[21]

Instructors typically develop PCK over time through experience. However, an individual's knowledge is often not shared between instructors or through peer-reviewed literature.[22] Our investigation of learners' representations of MOs emphasizes collective assessment knowledge and content knowledge of a community of practice to build collective PCK, which can then be used to develop instructional strategies to facilitate student learning of MO theory. Research shows that instructor explanations can minimize the development of alternative conceptions when such misunderstandings are anticipated and addressed.[23−25] Methodologies that uncover common errors and identify ideas that learners find particularly difficult may accelerate the process of improving the teaching of MO theory.

PREVIOUS RESEARCH ON STUDENT IDEAS USING MO THEORY

While there have been calls for more research into learner conceptions in advanced coursework (e.g., physical chemistry), little work has been done in inorganic chemistry.[26] Much of the work in inorganic chemistry has addressed other course topics that require visualization skills, such as molecular three-dimensional symmetry.[27−31] Research on student ideas about covalent bonding has focused on introductory ideas of ionic and covalent bonding with little attention to advanced bonding models.[13,14,32]

Taber found that pre-university students struggle to accurately interpret MO representations and typically do not choose to discuss bonding in terms of molecular orbitals.[16] Salah and Dumon asked students to describe covalent bonds and found that participants also did not spontaneously invoke MO concepts;[17] furthermore, they observed that learners at the end of their bachelor's degrees do not typically recognize that bonding MOs are lower in energy than the atomic orbitals that serve as their basis set.[17] Jenkins and Shoopman asked senior-level chemistry majors in inorganic chemistry to generate MO diagrams for multiple dioxygen species and use them to determine electron configurations and the relative stabilities of O_2^+, O_2, and O_2^-.[15] While students accurately constructed MO diagrams, Jenkins and Shoopman found that the majority of students could not use an MO diagram to predict the relative stability of the dioxygen species or use their MO diagrams to explain the information communicated in them. Strategic interventions in class improved student performance on a final exam, but Jenkins and Shoopman point out that incorrect inferences may result from students misapplying formulaic procedures that they do not fully comprehend.

We were unable to find any studies that have reported how students generate representations of molecular orbitals, and there are few examples in the literature of how students interpret these representations.

The study described herein asked students and instructors to generate representations of MOs and explain what information is encoded in their drawings. Generating representations and using them to explain phenomena are two of the skills that comprise one's representational competence.[33] Drawings can

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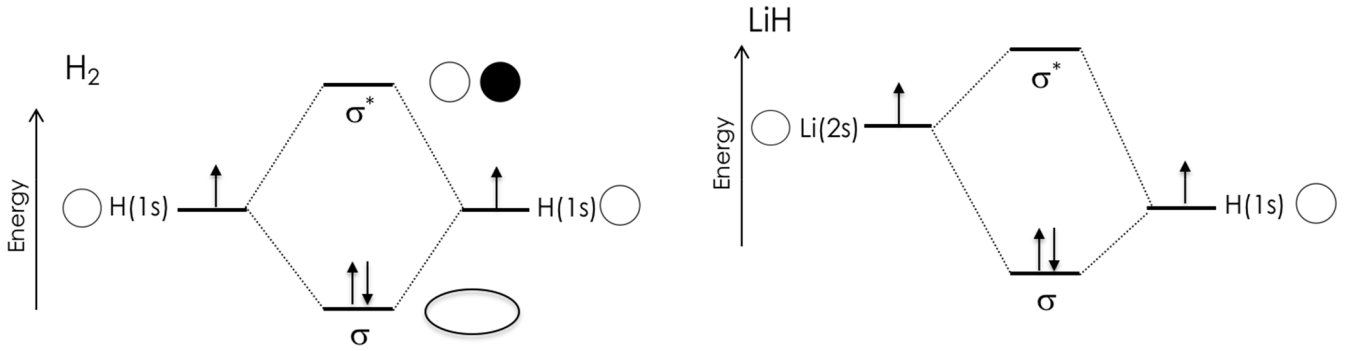

Figure 1. MO diagrams that were provided to students as part of the open-ended bonding question.

provide insight into the process students use to develop mental models, particularly when learners must explain why representations are appropriate for the given purpose or how they can be used to explain molecular behavior. Care must be taken when interpreting students' representations independent of explanations as students can get the "right answer" for the wrong reasons, such as by applying a set of rules or heuristics without any rationale.

By studying the representations of students and instructors from multiple institutions, commonalities and challenges in interpreting MO pictures were identified. Such an understanding contributes to the development of collective PCK about scientifically accepted MO representations.

METHODS

This work was approved by the Institutional Review Board (IRB) at Hope College or the IRB at each of the study sites.

Open-Ended Question Development

The data collection question used in this study was developed through an iterative process. Initially, 11 inorganic chemistry instructors collaboratively wrote an open-ended question to elicit a range of student responses. The initial question was tested with 99 students enrolled in postsecondary inorganic chemistry courses across five different four-year institutions. Preliminary analyses showed student responses focused on the construction and features of MO diagrams rather than on interpreting diagrams or making connections to properties (e.g., electron density). These findings limited our ability to understand the student conceptual understanding of MO theory. To address this, the question was iteratively revised based on pilot data to prompt students to provide responses that rely upon conceptual understanding;[34] this revision process included a team of six chemistry instructors who refined the question and tested it with an additional 13 students (version 2), 14 students (version 3), and finally 6 students (version 4) from a sixth four-year institution who had completed a course in inorganic chemistry and were participating in summer research. Only the data collected with the final version of the question are presented.

Classroom Use of the Open-Ended Bonding Question

The final revised question was provided to nine inorganic chemistry instructors from a range of institutions (four-year degree-granting through graduate degree-granting) who gave the question to students in their foundation-level inorganic chemistry course.

Instructors were given a copy of the open-ended question and told to have their students answer the question during class. Instructors were given autonomy in administering the question; however, they were advised to give students the question during their bonding unit any time after covering heteronuclear diatomic molecules. Instructors were advised to have students complete the question individually during class time. The research team provided several suggestions for how to administer and discuss the question after individual completion (e.g., as part of a think-pair-share, an individual activity followed by a whole class discussion, a quiz); ultimately the decision of how to administer the question was left to the instructors. The data analyzed for this study were drawn only from individual student responses prior to any in-class discussions or activities on the topic. De-identified, scanned copies of student responses were sent to the research team for analysis. Instructors also provided their own response to the open-ended question to demonstrate their idea of an ideal student response and provide context for their students' responses.

The complete final version of the question can be found in the Supporting Information (Figure S1). In this article, we analyzed student responses to the first part of the question, where students were given the orbital diagrams in Figure 1 and asked to respond to the following prompt: "Below are the molecular orbital diagrams for the H_2 molecule and the LiH molecule. (Energies are not to scale.) Draw/sketch the σ and σ^* molecular orbitals for the LiH molecule."

DATA ANALYSIS

The analysis focused on responses to the first part of the prompt: "Draw/sketch the σ and σ^* molecular orbitals for the LiH molecule." The coding scheme was iteratively developed by members of the research team, who reviewed student and instructor responses. The full coding scheme for the open-ended question can be found in the Supporting Information (Tables S1 and S2). While the second prompt asked students to explain the sketches of the MOs ("Using complete sentences, explain what information is provided by the drawings/sketches of the molecular orbitals in the H_2 and LiH molecules. Provide enough detail so that a fellow student has a good understanding of the information provided by the molecular orbitals."), student responses to this and other prompts in the open-ended question were often cursory and highly varied. This lack of consistency complicated our ability to make substantial assertions about student understanding. However, the large number of student sketches provided a rich data set for beginning our exploration of how students represent molecular orbitals.

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For our initial analysis, two researchers independently coded ∼10% of the data (19 responses). From this initial analysis, several codes did not agree; through discussion, the codebook was revised, with clarity and specificity added to code descriptions. With the revised codebook, the entire data set was coded by a single researcher. Of this independent coding, 10% was again discussed by the full research team to ensure agreement. This discussion led to minor modifications to the coding scheme, followed by a full recoding of the data. Our iterative coding process followed by a discussion of a subsample with the full research team occurred multiple times until all code discrepancies had been discussed and 100% agreement was achieved.

Because these data are reflective of 248 students from nine different institutions, the salient patterns and themes revealed by our analysis are more credible and transferable than results from data collected from a single classroom. This breadth of sampling, coupled with our iterative analysis process with multiple raters, adds trustworthiness to the findings.

RESULTS AND DISCUSSION

Our investigation explored how students sketched MOs of heteronuclear diatomic molecules. Figure 2 shows experimental shapes of LiH bonding and antibonding MOs as calculated in WebMO using the MOPAC semiempirical computational package with PM3 parameters.[35]

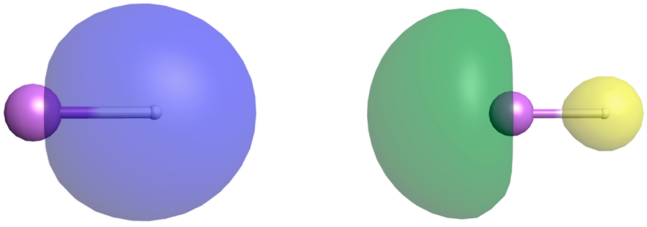

Figure 2. Bonding (left) and antibonding (right) MOs for LiH as calculated in WebMO using MOPAC/PM3. In both MOs, the lithium atom is on the left (purple sphere), and the hydrogen atom is on the right (white sphere). Contrasting colors are used to indicate opposite signs of the MO wavefunction, with red/blue or green/yellow being used for MOs that are occupied or unoccupied, respectively, in the ground state.

The σ bonding MO (Figure 2) results from the constructive interference of the lithium 2s and hydrogen 1s atomic orbitals; the MO does not contain a node and thus is shaded in a single color. Because the hydrogen 1s atomic orbital is lower in energy than the lithium 2s atomic orbital, it contributes more to the LiH bonding molecular orbital; this is reflected in the greater probability of finding the electron density on the right (hydrogen) atom. The σ bonding MO has significant electron density between atoms along the internuclear axis and is polarized toward hydrogen; there is low probability that the electron will be on the far side of the lithium nucleus.

The σ^* antibonding MO (Figure 2) results from the destructive interference of the lithium 2s and hydrogen 1s atomic orbitals. The σ^* MO contains a node along the internuclear axis, so the two lobes of the MO are shaded in different colors to indicate that the wavefunction has opposite signs in each region. The yellow and green coloring from WebMO indicates that this is an unoccupied MO. Because the lithium 2s atomic orbital is higher in energy than the hydrogen 1s atomic orbital, the 2s atomic orbital contributes more density to the σ^* antibonding MO; this is reflected by the greater probability of finding an electron near the lithium atom. For the antibonding MO, the electron density is primarily centered outside of the internuclear space.

The WebMO orbital calculations reflect the five criteria used to characterize responses to the prompt: (1) the atomic orbitals chosen, (2) the sign of the wavefunction in the MO, (3) the relative contribution of the atomic orbitals to the MOs, (4) the orbital overlap, and (5) the shape of the MOs.

Student and instructor drawings were individually evaluated for each of these five features. Representative drawings from participants that illustrate the coding dimensions are shown in Figure 3 and are discussed below. Additional examples of representations and how they were classified are in the Supporting Information.

Point 1: Most Students Chose the Correct Atomic Orbitals to Form the Molecular Orbitals of LiH

Respondents were asked to draw MOs of LiH. While students were not explicitly told which atomic orbitals to use as a basis set, the question prompt did identify the lithium 2s and hydrogen 1s atomic orbitals. We analyzed the drawings to identify whether students drew an s orbital (correct), a p or hybrid orbital (incorrect), an unidentifiable orbital (ambiguous), or no orbital (absence of a sketch). We note that while lithium's $2p_z$ orbital can be involved in bonding, we purposefully prompted students to employ a qualitative approach that considered only the 2s orbital. In some cases where students did not draw an orbital, they specifically wrote that the orbital "did not exist". Representative results are shown in Figure 4.

Unsurprisingly, all of the faculty and most students employed the correct basis set to construct MOs for LiH. A total of 91% of students selected s orbitals for the bonding MO and 84% of students selected s orbitals to construct the antibonding MOs. In some cases, students drew orbitals that included radial nodes for Li. Very few students chose incorrect orbitals (2% for both bonding and antibonding), and a small number drew orbitals that could not be interpreted (2% for both bonding and antibonding).

There was a difference in the number of students who did not sketch orbitals for the bonding and antibonding cases: 6% of students did not provide a drawing for the bonding MO compared to 13% for the antibonding MO. Several students wrote that the antibonding MO did not exist. We speculate that these students may think that only populated orbitals exist; an orbital without electrons, such as the unpopulated σ^* orbital, would therefore not exist. While not all students wrote this, we believe this may explain why more students did not draw antibonding orbitals compared to bonding orbitals.

Students with the alternative conception that unpopulated orbitals do not exist may have trouble understanding excited states and electronic transitions in molecules. Instructors should address and emphasize the significance of antibonding orbitals. Even though antibonding orbitals may not be populated, these orbitals represent how the electron density would be distributed in excited states. Additionally, antibonding orbitals may also be important for understanding reactivity; for example, low-energy empty orbitals may act as an acid (i.e., electron pair acceptor) in bond formation between a given acid and base.

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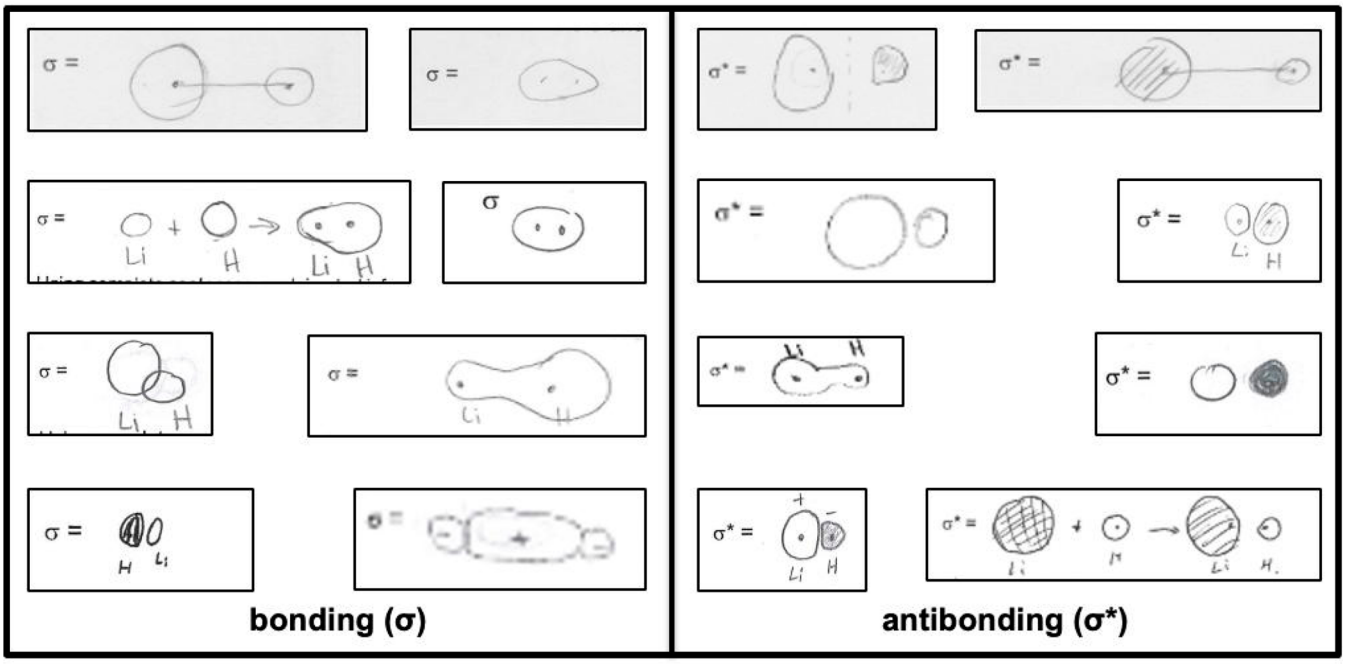

Figure 3. Representative student drawings of σ bonding (left) and σ^* antibonding (right) MOs for the LiH molecule. A complete set of exemplars and how they were coded can be found in the Supporting Information.

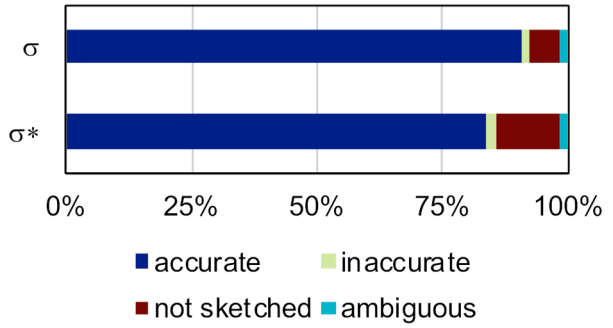

Figure 4. Student choice of basis set atomic orbitals in their representation of the bonding (σ) and antibonding (σ^*) MOs of LiH. In both cases, the respondents represented by dark blue used s orbitals to construct the MO (the scientifically accepted response). Those represented by green used incorrect orbitals (inaccurate). The respondents represented by red did not include a sketch of the molecular orbital (not sketched), and the respondents represented by light blue had drawn sketches that could not be interpreted (ambiguous).

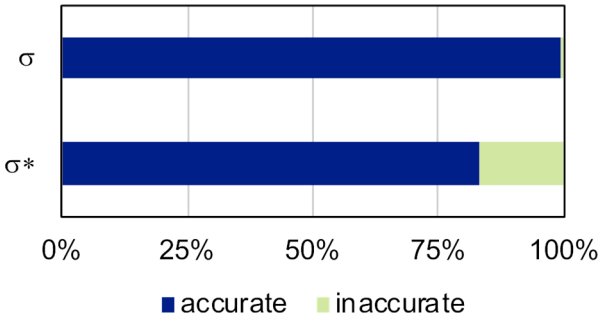

Figure 5. Student representations of the sign in the bonding (σ) and antibonding (σ^*) MOs of LiH. In both cases, the responses in dark blue are the percentage of responses with the scientifically accepted answer, and responses in green are the percentage of inaccurate answers. The σ bonding MO should be all one sign, and the two lobes of the σ^* antibonding MO should have opposite signs.

Point 2: Most Students Drew Molecular Orbitals That Show the Sign of the Wavefunction

When drawing molecular orbitals, inorganic chemistry textbooks use color differences, shading, or ± signs to show the different signs of the wavefunction. This is one way to understand whether a molecular orbital is bonding, nonbonding, or antibonding and to indicate nodes. In LiH, the bonding MO should have a single color, shading, or sign, while the antibonding orbital should show differences between the part of the orbital on Li and the part on H.

All instructors encoded the sign of the wavefunction using a scientifically accepted convention. However, there were significant differences in how students indicated sign in the bonding and antibonding MOs (Figure 5). While 98% of students showed the bonding orbital to have the same sign across LiH, only 83% showed the expected sign change in the antibonding orbital.

We attribute the increase in the number of incorrect sketches for the antibonding orbitals to students not realizing that the sign of the wavefunction is meaningful. Because our data were collected without opportunities to interview students, we do not know whether students recognize the information encoded in the sign of the wavefunction. However, we do see that most students recognize that including a wavefunction's sign in their sketches is important.

While the wavefunction sign is often overlooked, treated as arbitrary, or only tangentially mentioned in general chemistry courses, it is an important consideration when teaching orbitals in all courses irrespective of the placement in the curriculum. The wavefunction sign is an important concept for future study because it provides information about the number of nodes, which provides information about the orbital's relative energy. The presence of nodes also conveys information about the

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location of minima in the electron density. Orbital shape and symmetry provide information about allowed interactions in acid−base reactions, such as Lewis acid−base reactions and π-backbonding in metal carbonyls.

Point 3: Fewer than Half of Students Encoded the Atomic Orbital Contributions to Molecular Orbitals Correctly

For heteronuclear molecules, the relative size of each lobe in an MO is used to show the polarization of the electron density in the orbital. In general, the atomic orbital with the lower energy has a greater contribution to the bonding MO, shown by a larger size for that contribution relative to that of the higher-energy atomic orbital. The atomic orbital with the higher energy has a greater contribution to the antibonding MO. In LiH, the atomic orbital from hydrogen has a greater contribution to the bonding orbital. This can also be expressed by saying that the bonding MO has more hydrogen character, which means the electron density is polarized toward hydrogen. Conversely, the antibonding MO has more lithium character. If the antibonding MO were occupied, the electron density would be polarized toward lithium.

While all instructors sketched the antibonding orbitals using scientifically accepted representations, one instructor (11%) sketched the bonding orbital as having a greater contribution from lithium. Student responses (see Figure 6) showed greater variety.

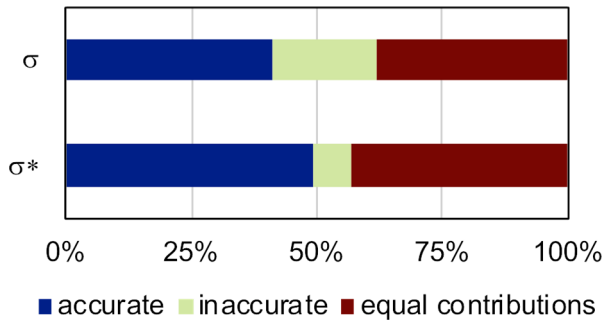

Figure 6. Student representations of the contribution of each of the atomic orbitals to the bonding (σ) and antibonding (σ^*) MOs of LiH. Responses in dark blue are the percentage of responses that provide the scientifically accepted response, in which hydrogen contributes more to the bonding MO and lithium contributes more to the antibonding MO. Responses in green are the percentage of inaccurate responses (i.e., lithium contributing more to the bonding MO or hydrogen contributing more to the antibonding MO), and responses in red are the percentage of drawings that displayed equal contributions from each atomic orbital.

Nearly half of the students sketched scientifically accepted representations of the bonding (41%) and antibonding (49%) orbitals, with the size of the hydrogen being larger in the bonding MO and the size of the lithium being larger in the antibonding MO. Others drew the two atomic orbitals as having equal contributions to the bonding (38%) or antibonding (43%) orbitals; thus, they did not demonstrate that the size of the orbital provides information about the distribution of electron density in the molecular orbital. A more interesting observation is that a larger number of students drew the lithium atomic orbital as having a larger contribution in the bonding MO (21%) than those who drew the hydrogen atomic orbital as having a larger contribution to the antibonding MO (7%); a single instructor also provided this response. One interpretation is that students attributed the relative size of the orbital lobes to the radius of the atoms rather than the electron density in the MO. Another interpretation is that students reversed the convention and thought that lower-energy orbitals contribute less.

The contribution of different atomic orbitals to molecular orbitals provides critical insights into the polarization of the electron density and dipole moments in molecules. This representation also provides information about the reactivity of molecules. For example, knowing that the highest occupied molecular orbital (HOMO) of CO is carbon-based explains why CO binds to a metal center through carbon rather than oxygen. Our findings support the result that students have difficulty connecting the concepts of electronegativity and polar covalent bonding.[36]

Point 4: Classic Representations of Molecular Orbitals May Interfere with Accurately Depicting the Overlap of the Orbitals

Another way to characterize the distribution of electron density in a molecular orbital is to look at how the atomic orbitals are drawn to show orbital overlap in the molecular orbital. In the bonding MO of a diatomic molecule, there is an increase in electron density between the two atoms, which is most accurately represented by showing the individual atomic orbitals fully merging into a single molecular orbital. In the case of the antibonding MO of a diatomic molecule, the representation should show a decrease in electron density between the two nuclei with a nodal plane (Figure 2).

All instructors correctly drew the antibonding orbital, while 22% of instructors drew a bonding MO that showed no orbital overlap. While this is inconsistent with calculations of electron density, this observation is consistent with some classic representations of MOs (e.g., Figure 7). Many classic texts

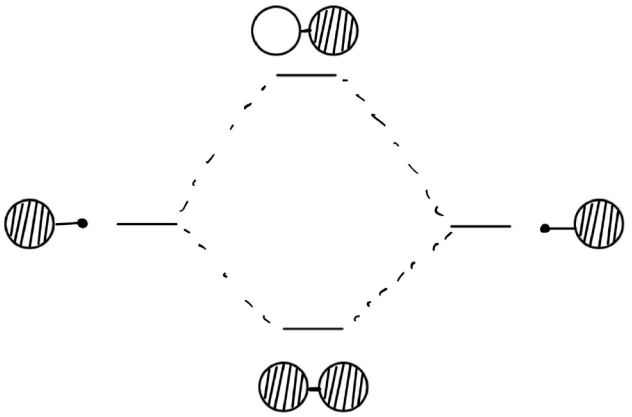

Figure 7. A classic MO representation for a homonuclear diatomic molecule.

and papers from the literature used hand-drawn graphics that are both easy to generate and meant to represent the coefficients of the linear combination of the atomic orbitals.[37−39] These images were used without considering how they could impact student interpretations. A chemist who was taught this way may not have knowledge of the currently accepted conventions for drawing MOs that help students associate the molecular orbital with the electron density. Alternatively, instructors may choose to use classic representations because they are quick and easy to sketch during real-time instruction.

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However, only using these representations in instruction risks students interpreting these drawings as actual MO shapes. Instructors who choose to use classic representations should emphasize that their primary value lies in communicating information about individual atomic orbital contributions to the molecular orbital and should stress that the relative size (or presence) of atomic orbitals in the diagram corresponds with coefficients in the MO wavefunction.

While student responses varied, most students drew a scientifically accepted representation of the orbital overlap in the bonding (72%) and antibonding (79%) MOs (Figure 8).

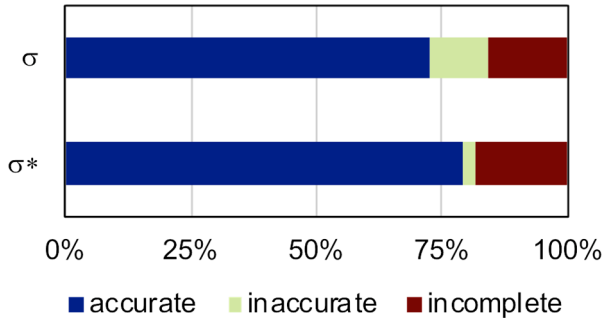

Figure 8. Student representations of the orbital overlap of each atomic orbital to the bonding (σ) and antibonding (σ^*) MOs of LiH. Responses in dark blue are the percentage of scientifically accepted responses, in which the bonding MO demonstrates enhanced electron density along the bonding axis, and the antibonding MO demonstrates a nodal plane between the two nuclei and an area of zero electron density along the internuclear axis. Responses in green are the percentage of drawings that failed to demonstrate the appropriate atomic orbital overlap. Responses in red are the percentage of drawings where two separate orbitals were drawn, but the orbitals either touched each other or were drawn as individual orbitals that overlapped.

For the bonding MOs, 12% of students drew orbitals with no overlap and 16% of students drew orbitals where there was incomplete overlap. Incomplete overlap refers to a drawing where two separate orbitals are drawn, but the orbitals either touch or are drawn as individual orbitals that overlap. Only 3% of students drew antibonding MOs as overlapping, while 18% drew orbitals with incomplete overlap.

These observations highlight the importance of explaining information encoded by molecular orbital overlap and how overlap is connected to electron density. Emphasizing orbital overlap provides an opportunity to discuss how the presence or absence of electron density between nuclei can stabilize or destabilize a bond.

Point 5: Molecular Orbital Shapes Often Depicted Non-Interacting Orbitals

In addition to the relative contribution of orbitals and their overlap, the overall shape of the MOs provides additional information about electron density. To fully represent the bonding MO of heteronuclear diatomic molecules, there should be not only a single region of electron density that is more localized on the lower-energy orbital (point 3 above) but also a region of enhanced electron density between the nuclei. Conversely, the antibonding MO should have a node between the nuclei (points 3 and 4 above) and have the electron density centered outside the internuclear space. Results describing how students represent the shape and distortion of the MOs are shown in Figure 9.

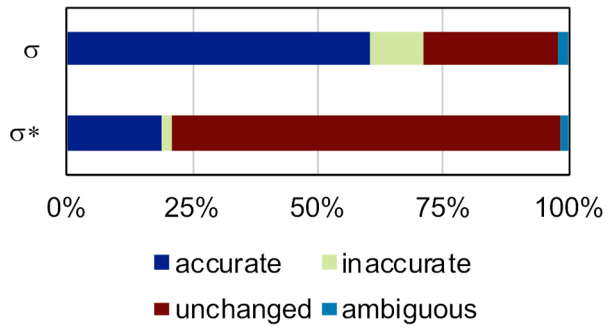

Figure 9. Student representations of the shape and distortion of the bonding (σ) and antibonding (σ^*) MOs of LiH. Responses in dark blue are the percentage of students who provided a scientifically accepted response, in which the bonding MO features enhanced electron density along the internuclear axis, and the electron density of the antibonding MO is centered outside of the internuclear space. Responses in green are the percentages of drawings that showed an inaccurate depiction of the electron density. Responses colored red are the percentage of drawings where the orbitals were undistorted when a bonding or antibonding interaction occurred. Responses colored light blue are the percentage of ambiguous responses that could not be classified.

There are many ways to draw the shape of molecular orbitals. For bonding MOs, in addition to the scientifically accepted drawing that showed increased electron density between the nuclei (61%), student drawings showed unchanged and undistorted atomic orbitals (27%), idiosyncratic representations where there was a partial merging of electron density between orbitals (11%), and ambiguous, uncharacterizable drawings (2%). Most drawings of the antibonding MOs depicted undistorted atomic orbitals (77%) while some showed the scientifically accepted representation where electron density is localized outside the internuclear space (19%). There were also idiosyncratic sketches that showed overlap between the atomic orbitals (2%) and ambiguous images (2%).

Nearly one-third of students drew the bonding MOs as discrete atomic orbitals. This could result from not understanding that electron density is shared between the two atoms or by mimicking an instructor or textbook representation. Students may not connect their drawings to the actual location of electron density in a molecular orbital. We believe that the large number of students who drew undistorted atomic orbitals for the antibonding case may be an artifact of a simplifying choice by instructors. Instructors may deem it sufficient to show that there is decreased electron density between atomic orbitals by having students draw undistorted atomic orbitals rather than showing that the electron density, particularly on lithium, is primarily outside the region between the nuclei. Instructors should consider how they draw these orbitals in light of their instructional goals.

Variation between Schools

There was variation between how students drew orbitals at the participating institutions. This variation can be seen in Figures S2−S6: while there was little variation in the choice of basis set (point 1) or the sign of the atomic orbitals that contributed to the MO (point 2), more variation was seen in the other ways students represented orbitals (points 3, 4, and 5). While it is not possible to link student responses with prior chemical knowledge, given the diversity of students in foundation inorganic chemistry courses (Table S3), these variations do

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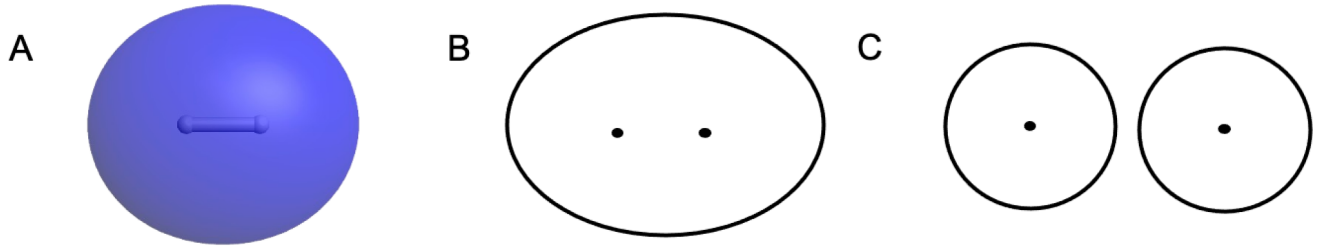

Figure 10. Inorganic textbooks use multiple representations of molecular orbitals. Common representations include (A) a 3D image approximating the electron density in a molecular orbital, as determined by a quantum mechanical calculation; (B) a projection of the 3D image into 2D space; and (C) individual orbitals that are combined through the LCAO approach.

not appear to be correlated with students' prior course experience, as identified by course prerequisites. We have several hypotheses for the variations observed between schools.

It is possible that the variation could result from differences in the emphasis of instruction. Students in our study were in courses that ranged from first-year courses with a single semester of general chemistry as a prerequisite to fourth-year courses with quantum mechanics as a prerequisite. It is reasonable to imagine that there are different instructional goals for these classes. Students are introduced to fewer dimensions of MO representations in the first-year class than in the fourth-year class. Representations are ultimately influenced by learning goals and instructional choices made by the instructor.

Another possibility is that students include representation dimensions used by their instructor. For example, at one institution, an instructor drew no overlap between either the bonding or antibonding orbitals; all students drew the same type of representation. However, at another institution, where the instructor drew no overlap in either MO, a mix of student representations was observed. It is possible that this instructor used multiple types of representations in their instruction. One of the authors of the article (B.A.R.) reflectively observed that while she begins instruction by using scientifically accepted representations, she often draws orbitals using the linear combination of atomic orbitals (LCAO) representation because they are easier to draw. In this study, we had no method of exploring whether students were drawing what they had seen from their instructor or another resource or if they fully understood the meaning encoded in their representations; however, these results still provide valuable information about the choices students make in their MO representations.

Representations in Textbooks

While we hope that students will develop representational competence, most textbooks do not help novice learners develop these skills. Inorganic chemistry textbooks use a range of representations when depicting MOs, but there are three common depictions in textbooks (Figure 10). The calculated three-dimensional (3D) MO wavefunctions (Figure 10a) and its two-dimensional (2D) projection (Figure 10b) are advantageous because they provide an approximation of the electron density in the molecular orbital that is consistent with quantum mechanical calculations. However, these can be more challenging to draw for larger molecules. A third representation that is derived from the LCAO approach, which shows how individual atomic orbitals combine to create MOs (Figure 10c), has a major limitation because it does not accurately depict the electron density as being delocalized across the molecule.

For experienced instructors, these depictions are rich in meaning; experts can easily translate between them and integrate their understanding of multiple representations. While instructors often assess students' representational competence, few instructors help students develop these skills.[40] A student with limited experience with MOs may have trouble interpreting these representations, let alone use them together to make inferences about chemical phenomena. Until students have linked meaning within and across these representations, they may draw sketches that mimic what they have seen before. Instructors and textbooks need to provide support for learners to help them interpret and translate across these representations.

The textbooks used by our participants approach MO theory from different perspectives and at different levels.[41−46] Of the textbooks reviewed for this paper, we have found only one that helps students develop representational competence by directly discussing how the different images are equivalent;[43] other textbooks do not provide explicit support that students may need to decode and link representations.

MO representations in online texts are also highly variable. Significantly, of the five criteria used to analyze sketches of molecular orbitals, only a single dimension is depicted consistently (the orbitals chosen as the basis set, point 1). The sign of the wavefunction (point 2), the relative contribution of atomic orbitals (point 3), how orbitals overlap (point 4), and the shape of the MOs (point 5) are not consistently illustrated. For example, in the Introduction to Inorganic Chemistry Wikibook chapter on molecular orbitals, multiple representations are used.[47] Figure 2.1.5 in this text inaccurately depicts points 4 and 5, while unnumbered figures in section 2.3 rely on classic representations that do not depict orbital overlap. Such misrepresentations may increase students' difficulty in attributing meaning to the representations. These misrepresentations have the potential to generate confusion and conflict; this is an opportunity for instructors to specifically address the affordance and limitations of multiple representations and highlight scientifically accepted representations.[33]

These observations again highlight the importance of helping students build representational competence to understand the meaning of the orbital representations while teaching MO theory so that students can fully assimilate the meaning we attribute to these orbitals and MO representations. This will, in turn, help students move from a novice understanding of MO representations toward a more scientifically accepted expert understanding. The variability seen is also a reminder of the importance of using consistent language and representations with novices.

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LIMITATIONS

A key limitation of this study was that data were collected as written responses to an open-ended question; there were no means to ask follow-up questions or request clarification of ideas and drawings. Therefore, we are limited in the claims we make about learner understanding, particularly in categorizing whether student responses are consistent with researcher interpretations of the data. Further research in this area would benefit from in-depth, think-aloud interviews to elicit deeper understandings of learner ideas, rationales, and generated drawings.

Despite this limitation, one of the study's strengths is that we analyzed responses across different institutions and from students at different stages in their programs. As such, despite our stated limitation, the multiple contexts in which data were collected add trustworthiness to the conclusions; salient ideas that crosscut the data are more meaningful, as they comprise multiple instructional and institutional contexts, making the findings more transferable than if only a single course or institution was studied.

CONCLUSIONS AND IMPLICATIONS

Our investigation into how students represent MOs serves as an opportunity for instructors to reflect on their own ideas about bonding and an array of student responses to improve the teaching and learning of molecular orbitals and MO theory. Instructors can be unaware of how the representations they use impact student understanding.[48−50] Bergqvist and Chang Rundgren have shown there is a link between how models are presented in textbooks and how they are used by teachers; they conclude that there is a need to bridge the gap between education research and teaching practices by developing teachers' PCK.[51] Our investigation helps build the collective PCK of molecular orbitals and MO theory by unpacking how learners represent MOs and the information encoded in these representations.

MO representations encode a large amount of information for experts that may not be obvious to novices. Findings from our analysis of learners' sketches of MOs show that students have incomplete understandings of the information encoded in MOs and may not attribute meaning to these representations in the ways experts do. The variability in responses between schools suggests that instruction impacts student ideas. Instructors need to help students correctly interpret molecular orbitals so that they can use these representations when they are encountered throughout the chemistry curriculum and in their chemical practice.

Using the consensus model of PCK,[52] we provide these recommendations for instructors. First, instructors should carefully consider their learning goals and identify the elements of molecular orbitals that are important for students in their contexts. Instructors may choose not to unpack all of the information encoded in MO representations, but these should be deliberate choices informed by specific instructional goals.

Second, using open-ended questions to elicit student ideas about molecular orbitals, such as the question used in this study (see the Supporting Information), can help instructors better understand student representations. In conjunction with class discussion, open-ended assessment items can provide a means for instructors to help students unpack information contained in representations and connect them with molecular properties (e.g., acidity, reactivity, and polarity). We are currently piloting instructional materials to help students develop deeper understandings of molecular orbitals, more conceptual understandings of chemical bonding, and an understanding of how to connect MOs with molecule properties.

Third, instructors should be careful with and question the representations used to depict molecular orbitals. When possible, they should use calculated MOs to help students visualize and ascribe meaning to MOs. Instructors should orient students to the different elements encoded in MO representations. They should also be explicit about the meaning of the sign of the orbital wavefunction, the size or contribution of the orbitals, orbital overlap, and orbital shape. Students do not attribute the same meaning to these ideas as instructors. Instructors can help students develop representational competence, which can further help them develop their conceptual understanding of bonding.[33,53,54]

Fourth, while our study focused on the teaching and learning of MO theory in inorganic chemistry, visualization and conceptualization of molecular orbitals is an important skill across all chemistry subfields. Instructors across the post-secondary chemistry curriculum need to guide students to better understand the representations that are used to depict molecular orbitals and to make connections with how molecular orbitals predict structure, properties, and reactivity.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.3c00823.

Codebook used to characterize drawings of the LiH MOs with exemplars, conceptual question completed by instructors and students as part of the research study, and graphs showing the variation of responses between participating institutions (PDF, DOCX)

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Author Contributions

B.A.R., J.L.S., and J.R.R. designed the study. B.A.R., M.M.K., J.L.S., J.R.R., and S.R.S. developed the conceptual question. B.A.R., M.M.K., J.L.S., J.M.P., and S.R.S. collected the data and conducted the data analysis. B.A.R., M.M.K., J.L.S., J.M.P., A.K.B., M.M.K., and S.R.S. discussed the data analysis, assisted in interpreting the results, and articulated implications of the results. B.A.R., J.M.P., J.L.S., and A.K.B. authored the paper. B.A.R., A.K.B., J.L.S., M.M.K., J.M.P., S.R.S., S.L., and J.R.R. reviewed and edited the paper.

Notes

The authors declare no competing financial interest.

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■ REFERENCES

(1) Marek, K. A.; Raker, J. R.; Holme, T. A.; Murphy, K. L. The ACS Exams Institute Undergraduate Chemistry Anchoring Concepts Content Map III: Inorganic Chemistry. *J. Chem. Educ.* **2018**, *95* (2), 233−237.

(2) Raker, J. R.; Reisner, B. A.; Smith, S. R.; Stewart, J. L.; Crane, J. L.; Pesterfield, L.; Sobel, S. G. Foundation Coursework in Undergraduate Inorganic Chemistry: Results from a National Survey of Inorganic Chemistry Faculty. *J. Chem. Educ.* **2015**, *92* (6), 973−979.

(3) Theobald, E. J.; Hill, M. J.; Tran, E.; Agrawal, S.; Arroyo, E. N.; Behling, S.; Chambwe, N.; Cintrón, D. L.; Cooper, J. D.; Dunster, G.; Grummer, J. A.; Hennessey, K.; Hsiao, J.; Iranon, N.; Jones, L.; Jordt, H.; Keller, M.; Lacey, M. E.; Littlefield, C. E.; Lowe, A.; Newman, S.; Okolo, V.; Olroyd, S.; Peecook, B. R.; Pickett, S. B.; Slager, D. L.; Caviedes-Solis, I. W.; Stanchak, K. E.; Sundaravardan, V.; Valdebenito, C.; Williams, C. R.; Zinsli, K.; Freeman, S. Active Learning Narrows Achievement Gaps for Underrepresented Students in Undergraduate Science, Technology, Engineering, and Math. *Proc. Natl. Acad. Sci. U.S.A.* **2020**, *117* (12), 6476−6483.

(4) Cooper, M. M.; Stowe, R. L. Chemistry Education Research—From Personal Empiricism to Evidence, Theory, and Informed Practice. *Chem. Rev.* **2018**, *118* (12), 6053−6087.

(5) Deslauriers, L.; McCarty, L. S.; Miller, K.; Callaghan, K.; Kestin, G. Measuring Actual Learning versus Feeling of Learning in Response to Being Actively Engaged in the Classroom. *Proc. Natl. Acad. Sci. U.S.A.* **2019**, *116* (39), 19251−19257.

(6) Freeman, S.; Eddy, S. L.; McDonough, M.; Smith, M. K.; Okoroafor, N.; Jordt, H.; Wenderoth, M. P. Active Learning Increases Student Performance in Science, Engineering, and Mathematics. *Proc. Natl. Acad. Sci. U.S.A.* **2014**, *111* (23), 8410−8415.

(7) Keller, M. M.; Neumann, K.; Fischer, H. E. The Impact of Physics Teachers' Pedagogical Content Knowledge and Motivation on Students' Achievement and Interest: Physics Teachers' Knowledge and Motivation. *J. Res. Sci. Teach* **2017**, *54* (5), 586−614.

(8) Baumert, J.; Kunter, M.; Blum, W.; Brunner, M.; Voss, T.; Jordan, A.; Klusmann, U.; Krauss, S.; Neubrand, M.; Tsai, Y.-M. Teachers' Mathematical Knowledge, Cognitive Activation in the Classroom, and Student Progress. *Am. Educ. Res. J.* **2010**, *47* (1), 133−180.

(9) Kunter, M.; Klusmann, U.; Baumert, J.; Richter, D.; Voss, T.; Hachfeld, A. Professional Competence of Teachers: Effects on Instructional Quality and Student Development. *J. Educ. Psych.* **2013**, *105* (3), 805−820.

(10) Gess-Newsome, J. Pedagogical Content Knowledge. In *International Guide to Student Achievement*; Hattie, J., Anderman, E. M., Eds.; Routledge, New York, NY, U.S., 2013; p 257−259.

(11) Baltieri, R. S.; Bego, A. M.; Cebim, M. A. Why the Covalent Bond Is Such a Complex Concept: A Conceptual Profile Proposal. *Int. J. Sci. Educ.* **2021**, *43* (12), 2007−2024.

(12) Hunter, K. H.; Rodriguez, J.-M. G.; Becker, N. M. A Review of Research on the Teaching and Learning of Chemical Bonding. *J. Chem. Educ.* **2022**, *99* (7), 2451−2464.

(13) Ozmen, H. Some Student Misconceptions in Chemistry: A Literature Review of Chemical Bonding. *J. Sci. Educ. Technol.* **2004**, *13* (2), 147−159.

(14) Ünal, S.; Çalık, M.; Ayas, A.; Coll, R. K. A Review of Chemical Bonding Studies: Needs, Aims, Methods of Exploring Students' Conceptions, General Knowledge Claims and Students' Alternative Conceptions. *Res. Sci. Technol. Educ.* **2006**, *24* (2), 141−172.

(15) Jenkins, J. L.; Shoopman, B. T. Identifying Misconceptions That Limit Student Understanding of Molecular Orbital Diagrams. *Sci. Educ. Int.* **2019**, *30* (3), 152−157.

(16) Taber, K. S. Compounding Quanta: Probing the Frontiers of Student Understanding of Molecular Orbitals. *Chem. Educ. Res. Pract.* **2002**, *3* (2), 159−173.

(17) Salah, H.; Dumon, A. Conceptual Integration of Covalent Bond Models by Algerian Students. *Chem. Educ. Res. Pract.* **2014**, *15* (4), 675−688.

(18) Jamieson, E. R.; Eppley, H. J.; Geselbracht, M. J.; Johnson, A. R.; Reisner, B. A.; Smith, S. R.; Stewart, J. L.; Watson, L. A.; Williams, B. S. Inorganic Chemistry and IONiC: An Online Community Bringing Cutting-Edge Research into the Classroom. *Inorg. Chem.* **2011**, *50* (13), 5849−5854.

(19) Shulman, L. S. Those Who Understand: Knowledge Growth in Teaching. *Educ. Res.* **1986**, *15* (2), 4−14.

(20) Magnusson, S.; Krajcik, J.; Borko, H. Nature, Sources, and Development of Pedagogical Content Knowledge for Science Teaching. In *Examining Pedagogical Content Knowledge: The Construct and its Implications for Science Education*; Gess-Newsome, J., Lederman, N. G., Eds.; Springer, Dordrecht, the Netherlands, 1999; p 95−132. DOI: 10.1007/0-306-47217-1_4.

(21) Rodriguez, J.-M. G.; Towns, M. H. Alternative Use for the Refined Consensus Model of Pedagogical Content Knowledge: Suggestions for Contextualizing Chemistry Education Research. *J. Chem. Educ.* **2019**, *96* (9), 1797−1803.

(22) Andrews, T. C.; Speer, N. M.; Shultz, G. V. Building Bridges: A Review and Synthesis of Research on Teaching Knowledge for Undergraduate Instruction in Science, Engineering, and Mathematics. *Int. J. Sci. Educ.* **2022**, *9* (1), 66.

(23) Diakidoy, I.-A. N.; Kendeou, P.; Ioannides, C. Reading about Energy: The Effects of Text Structure in Science Learning and Conceptual Change. *Contemp. Educ. Psych.* **2003**, *28* (3), 335−356.

(24) Wittwer, J.; Renkl, A. Why Instructional Explanations Often Do Not Work: A Framework for Understanding the Effectiveness of Instructional Explanations. *Educ. Psych.* **2008**, *43* (1), 49−64.

(25) Sánchez, E.; García-Rodicio, H.; Acuña, S. R. Are Instructional Explanations More Effective in the Context of an Impasse? *Instr. Sci.* **2009**, *37* (6), 537−563.
(26) National Research Council (U.S.). In *Discipline-Based Education Research: Understanding and Improving Learning in Undergraduate Science and Engineering*; Singer, S. R., Nielsen, N., Schweingruber, H. A., Eds.; The National Academies Press, Washington, D.C., U.S., 2012.
(27) Crandell, O. M.; Pazicni, S. Leveraging Cognitive Resources to Investigate the Impact of Molecular Orientation on Students' Activation of Symmetry Resources. *Chem. Educ. Res. Pract.* **2023**, *24* (1), 353−368.
(28) Nottis, K. E. K.; Kastner, M. E. The Effect of Instructional Modality and Prior Knowledge on Learning Point Group Symmetry. *J. Sci. Educ. Technol.* **2005**, *14* (1), 51−58.
(29) Luxford, C. J.; Crowder, M. W.; Bretz, S. L. A Symmetry POGIL Activity for Inorganic Chemistry. *J. Chem. Educ.* **2012**, *89* (2), 211−214.
(30) Southam, D. C.; Lewis, J. E. Supporting Alternative Strategies for Learning Chemical Applications of Group Theory. *J. Chem. Educ.* **2013**, *90* (11), 1425−1432.
(31) Dong, Y.; Zheng, S.-L. Resolving Space-Group-Choice Dilemma in Small-Molecule Crystallography for Chemistry Students Using Case-Based Learning Modules. *J. Chem. Educ.* **2021**, *98* (10), 3180−3188.
(32) Hunter, K. H.; Rodriguez, J.-M. G.; Becker, N. M. A Review of Research on the Teaching and Learning of Chemical Bonding. *J. Chem. Educ.* **2022**, 2451.
(33) Kozma, R. B.; Russell, J. Multimedia and Understanding: Expert and Novice Responses to Different Representations of Chemical Phenomena. *J. Res. Sci. Teach.* **1997**, *34* (9), 949−968.
(34) Cooper, M. M.; Kouyoumdjian, H.; Underwood, S. M. Investigating Students' Reasoning about Acid-Base Reactions. *J. Chem. Educ.* **2016**, *93* (10), 1703−1712.
(35) Polik, W. F.; Schmidt, J. R. WebMO: Web-based Computational Chemistry Calculations in Education and Research. *WIREs Comput. Mol. Sci.* **2022**, *12* (1), e1554 DOI: 10.1002/wcms.1554.
(36) Burrows, N. L.; Mooring, S. R. Using Concept Mapping to Uncover Students' Knowledge Structures of Chemical Bonding Concepts. *Chem. Educ. Res. Pract.* **2015**, *16* (1), 53−66.
(37) Albright, T. A.; Burdett, J. K.; Whangbo, M.-H. In *Orbital Interactions in Chemistry*; Wiley, Chichester, U.K., 2013.
(38) Jean, Y.; Volatron, F. In *An Introduction to Molecular Orbitals*; Burdett, J. K., Ed.; Oxford University Press, New York, NY, U.S., 1993.
(39) Cass, M. E.; Hollingsworth, W. E. Moving Beyond the Single Center-Ways To Reinforce Molecular Orbital Theory in an Inorganic Course. *J. Chem. Educ.* **2004**, *81* (7), 997.
(40) Popova, M.; Jones, T. Chemistry Instructors' Intentions toward Developing, Teaching, and Assessing Student Representational Competence Skills. *Chem. Educ. Res. Pract.* **2021**, *22* (3), 733−748.
(41) Rodgers, G. E. In *Descriptive Inorganic, Coordination, and Solid-State Chemistry*; Cengage Learning, 2002.
(42) Miessler, G. L.; Fischer, P. J.; Tarr, D. A. In *Inorganic Chemistry*, 5th ed.; Pearson, Boston, MA, U.S., 2014.
(43) Housecroft, C. E. In *Inorganic Chemistry*, 5th ed.; Pearson, Harlow, U.K., 2018.
(44) Weller, M.; Overton, T.; Rourke, J.; Armstrong, F. A. In *Inorganic Chemistry*, 7th ed.; Oxford University Press, Oxford, U.K., 2018.
(45) Pfennig, B. W. In *Principles of Inorganic Chemistry*, 2nd ed.; Wiley, Hoboken, NJ, U.S., 2022.
(46) Oxtoby, D. W.; Gillis, H. P.; Campion, A. In *Principles of Modern Chemistry*, 7th ed.; Cengage Learning, Belmont, CA, U.S., 2012.
(47) Introduction to Inorganic Chemistry/Molecular Orbital Theory. Wikibooks. https://en.wikibooks.org/wiki/Introduction_to_Inorganic_Chemistry/Molecular_Orbital_Theory (accessed 2023-08-09).
(48) Bergqvist, A.; Drechsler, M.; Chang Rundgren, S.-N. Upper Secondary Teachers' Knowledge for Teaching Chemical Bonding Models. *International Journal of Science Education* **2016**, *38* (2), 298−318.
(49) Taber, K. S.; Coll, R. K. Bonding. In *Chemical Education: Towards Research-based Practice*; Gilbert, J. K., Jong, O., Justi, R., Treagust, D. F., Driel, J. H., Eds.; Springer, Dordrecht, the Netherlands, 2003; p 213−234.
(50) Bergqvist, A.; Drechsler, M.; De Jong, O.; Rundgren, S. N. C. Representations of Chemical Bonding Models in School Textbooks-Help or Hindrance for Understanding? *Chem. Educ. Res. Pract.* **2013**, *14* (4), 589−606.
(51) Bergqvist, A.; Chang Rundgren, S. N. The Influence of Textbooks on Teachers' Knowledge of Chemical Bonding Representations Relative to Students' Difficulties Understanding. *Research in Science and Technological Education* **2017**, *35* (2), 215−237.
(52) *Repositioning Pedagogical Content Knowledge in Teachers' Knowledge for Teaching Science*; Hume, A., Cooper, R., Borowski, A., Eds.; Springer, Singapore, 2019. DOI: 10.1007/978-981-13-5898-2.
(53) Stieff, M. Improving Representational Competence Using Molecular Simulations Embedded in Inquiry Activities. *J. Res. Sci. Teach.* **2011**, *48* (10), 1137−1158.
(54) Stieff, M.; Lira, M.; DeSutter, D. Representational Competence and Spatial Thinking in STEM. In *Proceedings of International Conference of the Learning Sciences, ICLS*; International Society of the Learning Sciences (ISLS), 2014; Vol. *2*, p 987−991.

https://doi.org/10.1021/acs.jchemed.3c00823
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