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Conceptual Challenges Exhibited by Naïve Undergraduate Students in the Context of Atomic Orbital Energy Diagrams

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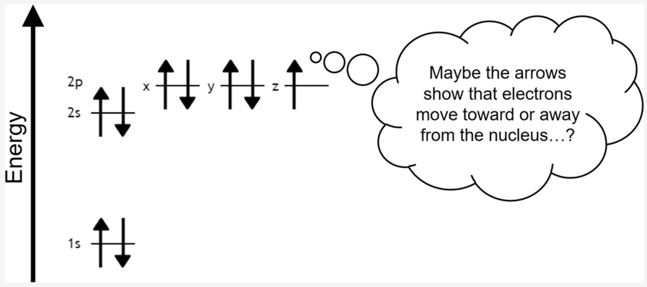

ABSTRACT: While visual representations are generally thought to help students learn chemistry, they can pose conceptual challenges. Arrows are a common visual feature used prominently across various visuals, such as energy diagrams. Although energy diagrams are widely used, research on what challenges arise in the context of energy diagrams is limited. To address this gap, the authors conducted interviews with 121 undergraduate students after they received instruction on atomic orbital energy diagrams. The interviews included two questions that served to get a broad sense of students' understanding of AOEDs and two questions that specifically focused on students' understanding of arrows that denote electrons. Students exhibited challenges in understanding electron motion by falsely assuming that electrons consistently follow a patterned motion. Further, students faced challenges understanding the energy of electron spin states and attractive and repulsive forces. These findings illustrate the need to investigate challenges that arise from implied meaning of various visual features of energy diagrams, which is key to developing instruction that helps students overcome challenges that arise in the context of energy diagrams.

KEYWORDS: *High School/Introductory Chemistry, First-Year Undergraduate/General, Chemical Education Research, Misconceptions/Discrepant Events, Atomic Properties/Structure*

Most chemistry instruction involves visual representations.[1−3] Visual representations play a critical role in chemistry education because many chemistry concepts cannot be directly observed even though they are highly visuospatial.[4,5] Hence, concepts are often taught via visual representations. What is more, instructors often assume that students have knowledge about concepts that are not explicitly taught by a visual representation but merely implied. Although visual representations are often considered to enhance students' learning,[6,7] they pose conceptual challenges,[8,9] such as, challenges in understanding concepts related to atomic structure.[1,10,11]

While prior research has documented students' conceptual challenges in the context of Lewis structures, shell models, lattice models, or electron pushing formalism,[10,12−14] energy diagrams are an under-researched type of visual representation. The present paper defines *energy diagrams* as a class of representation that shows the possible energy states of a chemical system (Figure 1). Within energy diagrams, orbital energy diagrams show the energy of orbitals and electron(s) in orbitals. *Atomic* orbital energy diagrams (AOEDs), which are the focus of the present study, depict the energy states of orbitals of multielectron *atoms*. Chemistry curricula[15] widely use AOEDs to illustrate how atomic structure relates to the energy levels of electrons in atomic orbitals, which has implications for bonding behavior, magnetic properties, and periodic table trends.

Although there are a variety of energy diagrams, they share several visual features, as illustrated in Figure 1. A prominent visual feature is the use of arrows. Generally, the exact meaning of arrows is not defined within the figure caption and is instead understood by prior knowledge of chemistry and chemical representation conventions. Across different types of energy diagrams, arrows can have different meanings (e.g., for transitions between energy states or electrons occupying energy states). Further, within a specific type of energy diagram, different types of arrows can stand for different constructs (e.g., a large arrow indicating energy level, with small arrows denoting electrons). This is particularly notable because prior research shows that chemistry students have difficulties assigning different meanings to different types of arrows.[14]

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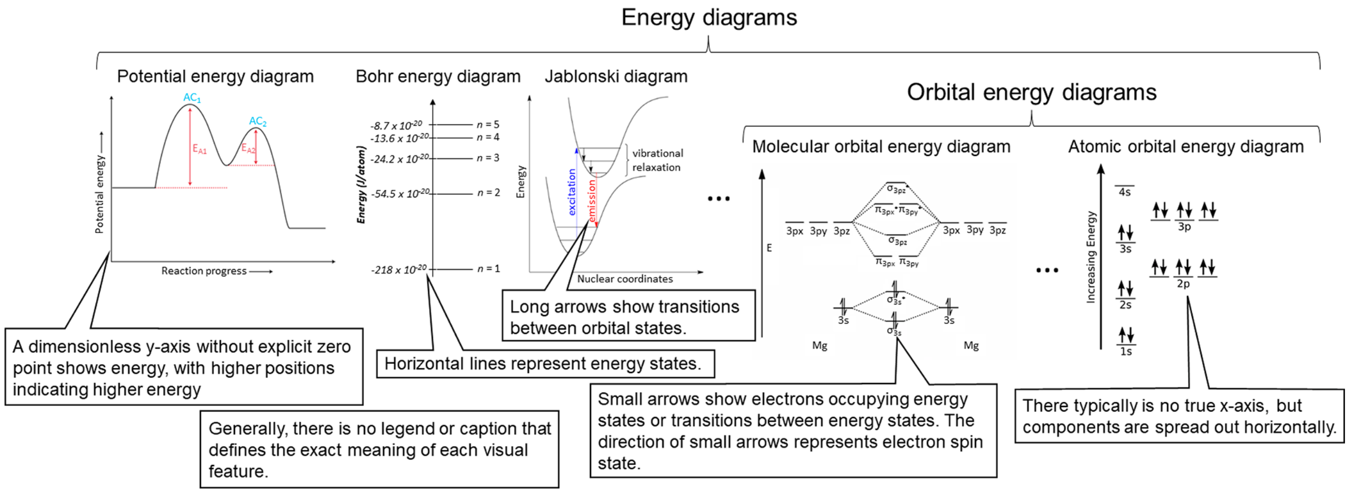

Figure 1. Types of energy diagrams.

Instruction related to energy diagrams broadly and AOEDs in particular is conceptually complex, as detailed below. This could create challenges for students' understandings of concepts that are explicitly shown by or implicitly invoked by energy diagrams. Instructors often fail to notice conceptual challenges related to visual representations.[8,16] A first step toward helping instructors address these challenges is to investigate which conceptual challenges arise in the context of instruction with a particular visual representation. To this end, this paper presents an interview study that investigates conceptual challenges that arise in the context of AOEDs among students who encounter AOEDs for the first time. While we document any challenges that became apparent in the interviews, our interviews placed a particular emphasis on students' interpretation of arrows that depict electrons.

■ THEORETICAL BACKGROUND

Learning with Visual Representations

Chemistry instruction centrally relies on visual representations to teach students about abstract concepts.[1−3,17] Researchers typically distinguish visual and symbolic representations.[8,18] Whereas symbolic representations have an arbitrary mapping to their referent (e.g., equations have no resemblance to the entity they describe), visual representations have similarity-based mappings to their referent. These similarity-based mappings make it easier for students to digest information[18,19] and can help students interpret symbolic representations.[6]

However, visual representations can be a source of confusion about concepts, in part for the very reason that the visual representation appears to give intuitive access to the concept. Students may assume that they understand a concept shown by a visual representation and tend not to question their understanding, especially when a concept is implied by the representation rather than explicitly described.[8] For example, as mentioned above, the meaning of arrows in energy diagrams is usually implied. Further, instructors often assume that students correctly understand concepts related to visual representations because they are obvious to themselves.[16]

To address this issue, research on representational competencies has investigated how to help students extract conceptual information from visual representations.[2,7,20] Representational competencies involve knowledge about how to map visual features to the concepts they depict.[6,18,21] For example, students presented with an AOED must map the small arrows to concepts related to electrons. Generally, research on support of representational competencies starts by examining which conceptual challenges arise in the context of a particular representation.[22]

Conceptual Challenges with Visual Representations

Prior research has documented students' conceptual challenges with visual representations. Much of this research focused on concepts that involve connecting macroscopic and submicroscopic phenomena that are illustrated by different representations.[23] For example, to understand chemical bonding, students need to understand what changes happen at the macroscopic level (e.g., changes to the reacting substances experienced in experiments or shown by pictures or videos), how these changes relate to the submicroscopic level based on the electronic configuration of each atom (shown by energy diagrams), the types of bonds that form (shown by orbital diagrams), the electronegativity distribution within the molecule (shown by electrostatic potential maps[24]), and the resulting spatial arrangement of the atoms in the molecules (shown by ball-and-stick figures). Challenges in understanding these concepts have been documented even among chemistry Ph.D. students.[25] This example illustrates that instruction around visual representations is conceptually complex.[26]

Numerous studies document conceptual challenges related to specific visual representations. For example, in the context of Lewis structures and ball-and-stick models, students exhibit challenges in understanding bonding when they falsely conceive of bonds as solid connections between atoms.[27,28] Such challenges can interfere with students' future learning about bonding,[29] about polarity and molecular geometry,[30] and about the relation between molecular structures and properties of substances at the macroscopic level.[31] Additionally and more specifically, prior research has revealed challenges related to understanding and using arrows in visual representations. Students have been shown to exhibit difficulties understanding how curved arrows show electron flow in reaction mechanisms, especially using arrows without understanding the underlying concepts.[14,32,33] However, little research has examined conceptual challenges with energy diagrams broadly or specifically with respect to their use of arrows.

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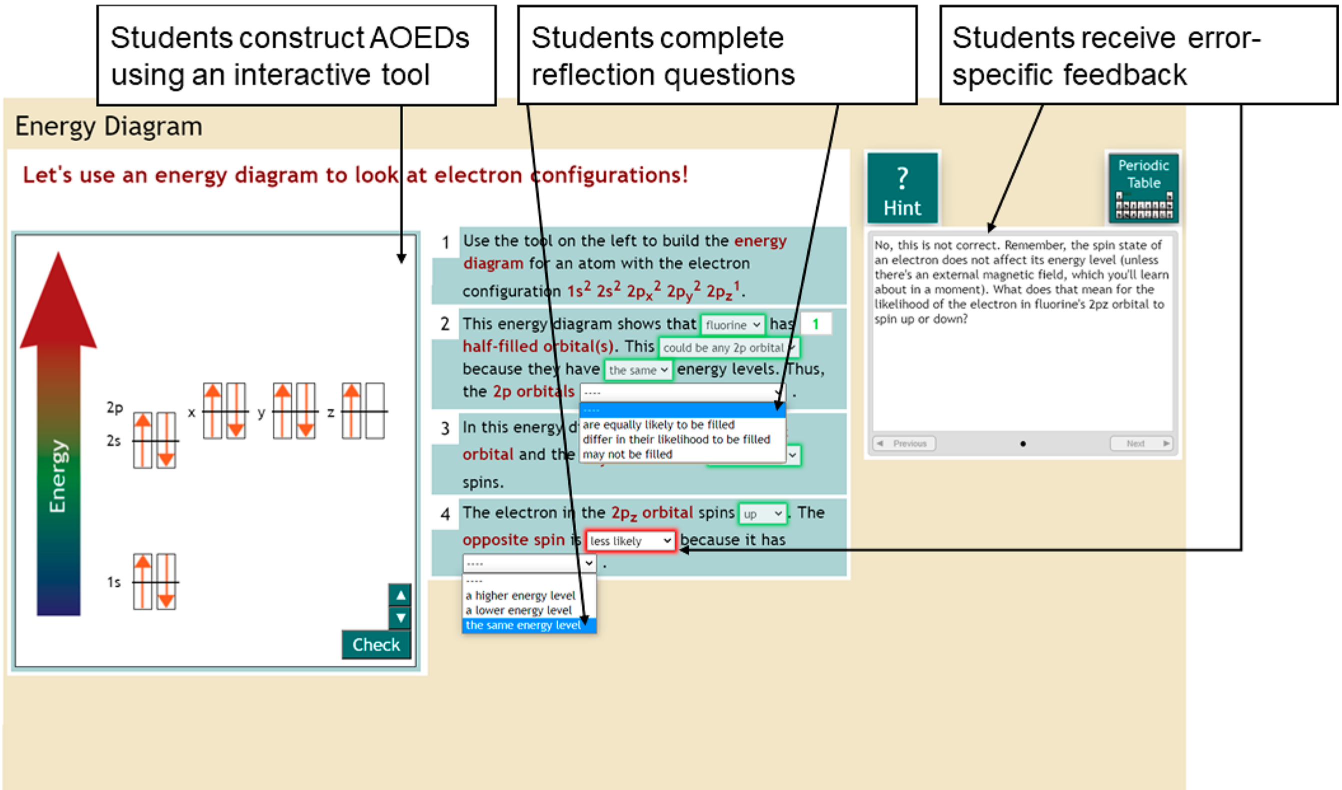

Figure 2. Example Chem Tutor problem.

Conceptual Challenges with Energy Diagrams

While prior research has not specifically investigated which conceptual challenges arise in the context of AOEDs, the literature documents two broader classes of conceptual challenges relevant to our work. A first set of challenges regards incorporating quantum mechanics concepts into students' understanding of chemical phenomena. Recall that AOEDs depict the energy states of electrons in orbitals, a function of proximity to the nucleus and the electrons' motion, which are quantum mechanical phenomena and concepts. More specifically, students often fail to distinguish concepts of quantum mechanics from classical mechanics.[34] For example, students often incorrectly describe electrons as moving according to some continuous translational motion consistent with classical mechanics.[12,35] Similarly, students often misconceive of the quantum mechanical phenomenon of spin as a classical mechanical phenomenon, describing electrons engaging in a rotational motion.[36]

A second set of challenges regards descriptions of subatomic particles. Students confuse "orbit", "orbital", "shells", and "subshells".[34−36] Further, students confuse "atom" and "molecule" or substitute them for one another.[12,28] These challenges can lead to miscommunications among students, teachers, and researchers and can impede students' ongoing conceptual learning.

Only a few studies have investigated conceptual challenges in the context of energy diagrams. First-semester general chemistry students using a Bohr energy diagram (Figure 1) fail to understand that an $n = 1$ shell has lower energy than an $n = 2$ shell, conceptual information that chemistry experts may find obvious.[37] To wit, the authors note that they "were not aware of [...] the amount of instructional guidance [...students] require" (p 82). Further, students using Bohr energy diagrams incorrectly understand the n value in Bohr energy diagrams as the number of electrons within the atom.[38] Finally, students have difficulties understanding energy states depicted in Jablonski diagrams (Figure 1).[39] Notably, none of these studies focused specifically on students' understanding of arrows depicting electrons.

■ RESEARCH QUESTION

Altogether, research suggests that conceptual challenges often arise around visual representations, including energy diagrams, but has not investigated which specific conceptual challenges arise in the context of AOEDs. Because prior research has focused on other specific types of energy diagrams (i.e., Bohr energy diagrams and Jablonski diagrams), focusing on AOEDs expands prior research to a less studied type of energy diagram. Further, AOEDs are typically used relatively early in the chemistry education sequence (i.e., in secondary school and early in general chemistry). Also, arrows are a prominent feature of AOEDs, which is shared by many other types of energy diagrams. Consequently, conceptual challenges with AOEDs broadly and with arrows in AOEDs specifically may appear among many students and could potentially persist over long periods or lead to confusion about other types of energy diagrams.

Thus, the present paper investigates the following: Which conceptual challenges do students exhibit after instruction with AOEDs?

To address this question, we recruited students who had no prior experience with AOEDs and atomic structure and interviewed them after they worked through instructional materials that used AOEDs to cover concepts related to atomic structure. The interview questions first probed their broad understanding of AOEDs and then focused on their understanding of small arrows that show electrons.

■ METHODS

Participants

Participants were recruited via email announcements, flyers, and posters, targeting students who had not taken any undergraduate chemistry classes to ensure they had no knowledge about atomic structure and energy diagrams. A screening verified that they were naïve to atomic structure and had no memory of prior exposure to energy diagrams. Specifically, students completed a survey asking them to list their major and prior chemistry education. They then took a pretest that assessed their knowledge about atomic structure and energy diagrams. Participants received $30.

Of 138 recruited participants, 17 were excluded (12 did not complete all portions of the study, and one had prior knowledge about atomic structure; for four, the intervention was not administered correctly), yielding a sample of $N = 121$ (84 female, 35 male, two undisclosed). They had an average age of 22.18 years (SD = 3.06) (eight undisclosed). Of the participants, 95.5% had taken high school chemistry, and 33.6% had taken advanced placement or honors chemistry in high school. Their average pretest scores were 8.5%, confirming that they were naïve to atomic structure and energy diagrams. Statistics on students' self-reported majors are available under Supporting Information.

Instruction

Students interacted with all instructional materials on a computer, using a type of educational technology for undergraduate chemistry: Chem Tutor.[4] Chem Tutor was designed on the basis of interviews with chemistry instructors and students and modeled after commonly used chemistry curricula.[22] Chem Tutor presented eight problems that used AOEDs to teach concepts related to atomic structure. Instruction was restricted to the orbitals of the ground state of the first 18 elements. In each of the eight problems, students created an AOED with a correct electron configuration and answered reflection questions. If students made a mistake in creating an AOED or in the reflection questions, they received feedback from Chem Tutor that provided conceptual information specific to their mistake (Figure 2).

The problems laid out key conventions of AOEDs: orbitals are shown as lines; the height of the line corresponds to the orbital's energy level; spatial orientations of orbitals are shown with the letters *x*, *y*, and *z*; arrows represent electrons; up and down arrows show electron spin. Further, the problems demonstrated chemical concepts related to the filling of orbitals: orbitals fill from lowest to highest energy; orbitals can have maximally two electrons; electrons in an orbital have opposite spin (Pauli exclusion principle); single electrons in orbitals of the same energy have matching spin (Hund's rule); and electrons fill orbitals of the same energy with a single electron before orbitals fill with a second electron. Additionally, the problems challenged students to consider a few ways orbitals or electrons therein might be of equal energy and thus equally likely to have a certain electron configuration, as well as an exception when an atom is in an external magnetic field and electrons whose spin state aligns with the field are of lower energy. Finally, the problems asked students to consider the definition of key terms and how those terms applied to the filling of AOEDs (e.g., spin state, valence electron).

Assessments

Students completed a pretest, an immediate posttest directly after instruction, and a delayed posttest (3−6 days after instruction; results from the tests are reported elsewhere[40]). Interviews, lasting 5−10 min, were conducted after each posttest. The AOED was not visible during the interview because we were interested in students' mental models (i.e., internal representations) rather than an explanation of the external representation. The first two interview questions served to get a broad sense of students' understanding of AOEDs. To this end, students were asked how an AOED represents an atom, and how an AOED shows the energy of electrons in an atom. Subsequently, two questions focused on the meaning of arrows denoting electrons in AOEDs. Specifically, students were asked what the up and down arrows represent; and what determines whether an arrow points up or down. The interviewer used a semistructured approach by asking students to elaborate on aspects of their explanation if they provided short answers or did not address the posed question. Inaccurate responses by the student were not probed further. The full interview protocol is available under Supporting Information.

Analyses

After transcribing the interviews, the authors used a constant comparative method to identify and understand challenges in students' understanding of the concepts taught with AOEDs.[41] While a detailed description of the constant comparative method is beyond the scope of this paper, our process involved comparing instances of conceptual challenges to one another until distinct categories emerged. Specifically, the first author used 50% of randomly selected interviews to compare interview responses within and between categories. This served to characterize the categories and develop a coding scheme that described eight recurring challenges. Our use of the constant comparative method did not specifically focus on challenges related to arrows but aimed to reveal any type of challenge that students' responses to the interview questions revealed. Next, the first author worked with another coder to reach consensus about how to apply the codes to the transcripts. Then, the coders independently coded randomly selected transcripts in increments of 10%. Disagreements were discussed, and the coding scheme was clarified if needed. Then, they independently coded 10% of the data, achieving an interrater reliability of $\kappa = 0.71$, which is considered substantial agreement in behavioral sciences. The first author then coded the remaining transcripts.

■ RESULTS

To investigate which conceptual challenges students exhibit after instruction with AOEDs, the authors examined the codes that emerged from the interviews. The following description first explains the concept or phenomenon that proved challenging and then describes the challenges students exhibited. Table 1 provides an overview of the prevalence of these conceptual challenges per student (i.e., counting how many students exhibited the challenge at least once) and in total (i.e., counting how many times the challenge was mentioned, allowing for multiple occurrences per student).

Electron Motion

While AOEDs do not explicitly describe electron motion, they visualize related phenomena, including orbitals and spin state.

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Table 1. Conceptual Challenges Sorted by Prevalence

Misconception	Number of Participants Who Exhibited the Challenge at Least Once	Total Number of Occurrences of Challenges across Participants/Interviews
Electron motion (EM)	76 (63%)	142 (15%)
EM-orbiting	28 (23%)	46 (5%)
EM-unspecified axis	21 (17%)	27 (3%)
EM-independent axis	19 (16%)	33 (3%)
EM-proximity	11 (9%)	25 (3%)
EM-other	15 (12%)	20 (2%)
Orbital spin energy	33 (27%)	50 (5%)
Incorrect language	21 (17%)	56 (6%)
Wrong orbital order	17 (14%)	21 (2%)
Ground state	11 (9%)	23 (2%)
Valence electron	9 (7%)	11 (1%)
Attraction/repulsion	7 (6%)	13 (1%)
Bad example	4 (3%)	5 (1%)
Total	121 (100%)	963 (100%)

Orbitals do not describe an electron's location but a mathematical function that can be used to calculate the probability of finding an electron at a particular location relative to the nucleus. Spin state does not describe electron motion but a magnetic field that exists due to an intrinsic angular momentum that has no equivalent in the classical mechanical world.

There were 78 students who exhibited challenges in understanding electron motion ("electron motion (EM)"). The authors further categorized these challenges based on how students described electron motion.

First, 29 students described electron motion as circling around the nucleus ("EM-orbiting"). For example, Charlie described that electrons are "orbiting around the nucleus." (Student names are pseudonyms.) Some students, like Charlie, described a literal orbit where the electron spins around an internal axis and around the nucleus. Others merely described rotating around the nucleus.

Second, 21 students described electron motion as consistently rotating without specifying around what axis the electron spins ("EM-unspecified axis"). For example, Meili explained that the up and down arrows represented "the spin of the electron, but I don't really know what it's... spinning around."

Third, 20 students described electron motion as consistently spinning or rotating around an axis of rotation particular to the electron ("EM-independent axis"). For example, Alejandro explained that each arrow in the AOED "represents how the electron spins around its own axis, whether it's spinning clockwise for an up spin or counterclockwise for a down spin."

Fourth, 11 students described electrons as having a consistent transverse motion toward or away from the nucleus ("EM-proximity"). For example, Jaidyn explained that the AOED shows "whether or not, like, they're moving towards or away from the nucleus."

Finally, 15 students described other consistent patterns of motion that did not recur across other students ("EM-other").

Orbital Spin Energy

AOEDs depict electron energy levels. Up and down spins are of equal energy and hence equally likely. Therefore, it does not matter whether the first electron in an orbital is an up or down arrow. There are two exceptions pertinent to this study. First, when multiple orbitals have equal energy, each orbital has one electron of a matching spin before any orbital is filled with a second electron (Hund's rule). Second, if an external magnetic field is applied to the atom, the spin state that aligns favorably with that field has lower energy.

There were 33 students who exhibited challenges in understanding orbital spin energy. Some students explicitly said spin states differed in energy. For example, Gifty said, "when [electrons are] paired in twos, one faces up and one faces down because they have slightly different energy levels." Other students implied a difference in energy when discussing orbital filling order. For example, Edna noted, "if there is no external magnetic force then [the orbital] usually starts with an up spin, and if there is an external magnetic force then it starts with a down spin."

Incorrect Language

When working with AOEDs, students encounter technical vocabulary that includes words related to atomic structure (e.g., protons, neutrons, and electrons). Further, several keywords describe electrons and their behavior: Electrons move in orbitals. Each orbital can hold maximally two electrons. Within an orbital, electrons must have opposite spin (Pauli exclusion principle).

There were 22 students who exhibited challenges in using technical language. Some students used the term "orbit" instead of "orbital". For example, Hunter explained, "in each orbit there are two electrons which have opposite mag, eh, magnetic state." Other students called the nucleus "nuclear." Some students incorrectly used the term "molecule" instead of "atom". For example, Ankit said, "pick your molecule on the table of elements." Finally, some students stated that the electron exclusion principle was attributable to Bernoulli rather than Pauli.

Wrong Orbital Order

AOEDs are used to teach students about orbital order. Orbitals closer to the nucleus have lower energy. Further, orbitals fill from lowest to highest energy (e.g., 1s before 2s).

There were 17 students who exhibited challenges in understanding or recalling atomic orbital order. Some students left out specific orbitals when enumerating them. For example, Galih explained that orbitals "are filled going from 1s to 2s to, eh, 3p and so on," leaving out the 2p and 3s orbitals. Other students left out an energy level or orbitals of a certain principal quantum number. However, other students mentioned orbitals that do not exist. For example, Kai listed the "1s, 1p, 2s, 2p, 3s, to eh 3p" orbitals, adding 1p orbitals, which scientifically do not exist. Further, students stated that p orbitals are lower in energy than s orbitals. For example, Loren related the energy level of atomic orbitals to the periodic table, suggesting, "if you go on the, the far left of the periodic table that's the s column, and [...] the next column you're gonna get is the p column, em, and the p column has a little bit less energy." Finally, some students described orbitals that are closer to the nucleus as having higher energy. For example,

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Scout explained, "the bottom of an energy diagram represents the lower energy electrons that are farthest away from the atom's nucleus."

Ground State

Text accompanying AOEDs often mentions that an atom is shown in its ground state. The ground state is the lowest energy state of a chemical system.

There were 11 students who exhibited challenges in understanding the term "ground state". Some students thought that the ground state meant that an atom is not in a magnetic field. For example, Robin explained that spin state is determined by whether "the electron is in ground state or if there's a magnetic field attached to it." Other students thought ground state meant an atom is not in an ionic state. For example, Levi noted, "the ground state means it has to have the same amount of protons as electrons."

Valence Electron

AOEDs depict valence electrons, which are electrons in an atom's highest occupied energy level.

There were 10 students who exhibited challenges in understanding valence electrons. Some students thought all electrons are valence electrons. For example, Asher explained, "the first orbital- two valence electrons, em, and the second orbital can also hold two valence electrons up to, em, as many electrons are attached to the atom," not differentiating between electrons in the 1s and 2s orbitals. Other students thought a valence electron is the second electron in an orbital. For example, Ankit explained, "the valence electron in that orbital will then be the opposite of whatever the first one was." However, other students thought that valence electrons are unpaired electrons. For example, Elvan elaborated, "if it's a pair of electrons one has to spin up, one has to spin down, but if it, like, a valence electron I think it can be like either." Finally, some students suggested that an atom may not have valence electrons. For example, Elia said, "if there is no valence electrons then every, eh, orbital has to have one pointed upward and one pointed downward."

Attraction/Repulsion

AOEDs can be used to discuss electrostatic and magnetic forces of attraction and repulsion among subatomic particles. Electrons are attracted to protons, and electrons repel one another due to electrostatic forces. Further, several magnetic forces are relevant to AOEDs. First, up or down spin states are magnetic fields arising from electron motion and are usually of equal energy. Second, when an external magnetic field is applied to an atom, the atom will orient such that the magnetic moments of its electrons align with the external field. Because the two spin states are opposites, the electrons are then aligned or antialigned with the external magnetic field and are slightly different in energy. Atoms will orient such that the greatest number of electrons are aligned favorably with the external magnetic field.

Seven students exhibited challenges in understanding attractions or repulsions by subatomic particles. Some students thought that electrons are not always attracted to the nucleus. For example, Arya stated, "the electron is, is being attracted to either the outside electromagnetic force or the nucleus" and "one [electron] is being, em, attracted to the nucleus, and because electrons repulse each other, the other one is therefore going the opposite direction." Other students suggested that electrons do not universally and permanently repel one another. For example, Jaidyn explained, "electrons are supposed to repel each other, but then I think if there is something involved it makes them not repel." However, others thought electrons attract one another. For example, Madison said, "the, em, electrons attract to each other rather to form the atom."

Bad Example

When asked to draw an AOED, students may be asked to choose a suitable example element.

Four students exhibited challenges in presenting example elements by incorrectly stating how many electrons an atom of a particular element has. For example, Arya said: "An energy diagram essentially shows the placement and the amount of electrons that a certain atom has. So, it's like, for example, I think nitrogen has four."

■ DISCUSSION

The present paper investigated which conceptual challenges naïve students exhibit after instruction with AOEDs. Our interview study probed students' broad understanding of AOEDs while also focusing on students' understanding of a particular visual feature: arrows. The following discussion examines how the identified challenges relate to those documented in prior research, what might give rise to the challenges, and potential implications for teaching.

Challenges Identified in Prior Research

The challenges related to electron motion identified here align with what Nicoll[28] called microscopic misconception of motion, which describes "all types of motion, including the motion of molecules, atoms, and/or electrons," including solar system analogies as documented elsewhere.[12,34] In contrast to this prior research, the present study specifically focused on AOEDs. Hence, the present findings extend prior research by showing that these misconceptions are pervasive when working with energy diagrams. This is notable because energy diagrams do not invoke a solar system metaphor through their design (as opposed to shell models, for example, which do). Further, the present paper relates this challenge to a larger phenomenon of challenges regarding understanding electron motion.

Additionally and more specifically, the EM-unspecified axis and EM-independent axis challenges, which describe inaccurate ideas about electrons moving in a patterned circular motion, are similar to Taber[36] who noted that students "associate the term "spin" with the macroscopic phenomenon of that name." Expanding on Taber's work, the present study shows that students can experience multiple such conceptual challenges simultaneously.

Further, previous research has noted that students do not know the correct filling order of atomic orbitals. Much like the "wrong orbital order" challenge identified here, Taber[36] found that students incorrectly identified the filling order of atomic orbitals, although Taber's study did not involve energy diagrams. The present study suggests that, by making the relationship between energy level and average distance from the nucleus salient, AOED can make this challenge apparent.

In addition, challenges in understanding attraction/repulsion have been discussed elsewhere. Nicoll[28] observed that "students tried to explain chemical bonding in terms of electrons attracting one another." Although the present study did not focus on bonding, it revealed related challenges, including inaccurate ideas of electrons within an atom being attracted to one another. The overlap between the present

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findings and Nicoll's findings suggests that challenges in understanding electron attractions are prevalent across topics.

Additionally, the present study yields novel insights into challenges in using technical terms, which is in line with studies in in other contexts, with other populations, and with other representations.[12,35]

Finally, we note that the challenges identified here are different from the conceptual challenges and barriers to learning previous researchers have found among students working with arrow pushing formalism. Nevertheless, students' difficulty using or explaining arrows properly made conceptual challenges similarly salient across studies. Previous work described students' challenges in correctly using and explaining curved arrows, which called attention to students' poor understanding of principles previously taught (such as acid/base chemistry),[14] their lack of recognition that the principles need to be used when using arrow pushing formalism, and their inability to use the formalism to predict or rationalize chemical behavior.[42] Similarly, the explanations of the meaning of arrows from the students in the present study call attention to students' misunderstandings of electrostatic and magnetic attractive and repulsive forces, principles generally taught in primary and secondary school, cataloged in *attraction/repulsion*. The fact that analysis of arrows in AOEDs gave rise to awareness of new conceptual challenges speaks to the value of researching students' learning using visuals in multiple contexts and populations, especially the visually or conceptually more complicated aspects of visuals, such as arrows.

In sum, several of the challenges identified here have been shown in other contexts, suggesting that they are not necessarily *caused* by AOEDs but *become visible* when students work with AOEDs. Further, the present study extends previous findings by documenting these challenges among a different context and population. In contrast, several of the challenges identified here have (to our knowledge) not previously been documented, including challenges that involve inaccurate ideas of electrons having constant motion toward or away from the nucleus and of spin states having different energies. It is possible that some aspects of these challenges may have arisen from the specific design of the AOED and instruction related to the AOED, as discussed next.

Challenges Potentially Arising from the AOED and Related Instruction

It is plausible that four of the challenges identified here, three of which relate to the use of arrows to represent electrons, may arise from the design of AOEDs. First, this use of arrows may give rise to the EM-proximity challenge. Recall that the vertical height of the orbitals roughly corresponds to distance from the nucleus because this distance is proportional to its energy. From this perspective, the up and down arrows literally point toward or away from the nucleus. This visual feature may induce the idea that electrons are moving toward or away from the nucleus.

Second, this use of arrows might reinforce challenges in understanding attraction or repulsion between electrons and nuclei. If students have prior inaccurate ideas about attraction/repulsion, visual cues suggesting that electrons move toward or away from the nucleus could reinforce them.

Third, the common practice of showing the up arrow first and on the left of an orbital may give rise to challenges in understanding the energy of spin states. The textbooks reviewed for this study show the up arrow first, even though there is no rule that the up spin electron shown with an up arrow should be drawn first. Generally, chemists are taught that both spins have equal energy, so choosing when to draw each arrow in the diagram is arbitrary. However, it is possible that repeated exposure to one option subliminally teaches students to think the up spin is lower in energy.

Fourth, it is possible that AOEDs reinforce existing challenges in understanding the term "valence electron". AOEDs often show core electrons as well as valence electrons at multiple heights, so height does not visually differentiate core electrons from valence electrons. Thus, if students have previous inaccurate ideas about valence electrons, the AOED may reinforce them.

In addition, it is plausible that three ways in which AOEDs are taught may give rise to some of the challenges identified here. First, four challenges implied a circular motion (i.e., EM-orbiting, EM-unspecified axis, EM-independent axis, and some of EM-other). In part, this may result from the term "spin", which is a historical misnomer that implies a literal rotation. Additionally, this may result from the use of analogies of objects literally spinning when explaining the concept of electron spin, which was common in the textbooks reviewed for this study. Textbooks vary in how explicitly they address that the example is an analogy and not a physical reality.

Second, challenges in understanding valence electrons may arise because of the multitude of sometimes oversimplified rules students have to learn when constructing an AOED. Some students' incorrect definitions of valence electrons conflated some of these rules. To illustrate, consider Ankit who thought the valence electron is the second electron placed in an orbital, or Elvan who thought valence electrons are unpaired electrons. When learning to draw an AOED, students learn about Hund's rule, the Pauli exclusion principle, and other visualization conventions. Having to learn the definition of valence electrons (or to rethink a previous incorrect definition) might be overwhelming and lead to conflations as in Ankit's and Elvan's cases, especially given that AOEDs do not visually differentiate valence and core electrons.

Third, it is possible that teaching practices around AOEDs give rise to challenges in understanding attractive and repulsive forces. AOEDs can be used to teach students about electrostatic attractive/repulsive forces of atomic components, magnetic attractive/repulsive forces resulting from the motion of atomic components, and the magnetic attractive/repulsive forces resulting from a hypothetical external magnet. Teaching these concepts simultaneously could be overwhelming and lead to conflations of electrostatic and magnetic forces. To illustrate, consider Arya and Jaidyn, who included a mix of these forces in their explanations.

Implications for Teaching

Being aware of challenges that arise in the context of a particular visual representation is a first step toward helping students acquire representational competencies and in addressing potential inaccurate ideas. First, it may be useful to teach not only the concepts that are explicitly shown by AOEDs but also to teach explicitly conventionally used visual features that imply concepts that students may misunderstand. Our results suggest that arrows denoting electrons are a visual feature that poses challenges to students that should be explicitly addressed. Other visual features that our interviews did not probe specifically could include the chemical meaning of lines denoting orbitals and other limitations and inaccuracies

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of the diagram (e.g., half-filled p orbitals are shown as degenerate with empty p orbitals for simplicity even though they are not). Second, it could be helpful to address directly the conceptual challenges described here, for example, by explaining that AOEDs do not consistently or accurately represent an orbital's average or mode distance from the nucleus. Third, it might be helpful to avoid using analogies of spinning macroscale objects to teach spin. Fourth, teachers could consider demonstrating AOEDs where the down arrows are shown first or on the left with equal frequency to address challenges in understanding spin states and inaccurate ideas such as the up spin having lower energy.

Improved practices around teaching with AOEDs could be impactful because AOEDs are among the energy diagrams taught earliest to students and because other types of energy diagrams depict related chemical concepts using many shared visual elements. Thus, this could help mitigate not only the challenges identified here but also other challenges that might arise as students work with closely related energy diagrams. Such challenges could arise in later instruction when students learn about more nuanced spin state rules, more complicated orbital energy diagrams that include d orbitals, or degenerate ground states. Finally, educators who teach more advanced students should be aware that they may have to address some of the challenges identified here.

LIMITATIONS

Our findings should be interpreted in light of several limitations. First, half of our interview questions focused on one particular visual feature, namely, arrows denoting electrons. There are a multitude of other visual features (e.g., the arrow on the vertical axis of the energy diagram, lines showing orbitals) that may pose additional challenges for students. Thus, the challenges identified here are likely not exhaustive of all challenges posed by AOEDs. Our hope is that this study increases awareness that AOEDs contain potentially confusing visual features that are worth exploring in future research that focuses on additional visual features.

Moreover, while our choice of conducting the interviews without the AOED was intended to reveal insights into students' mental models, it is possible that additional or different challenges would arise in interviews where the AOED is presented to students. Future research on additional visual features should hence be conducted with and without AOEDs present during the interviews.

In addition, the present study purposefully recruited students without prior exposure to energy diagrams because the goal was to investigate which conceptual challenges students exhibit after students' first exposure to energy diagrams. This choice enhances the internal validity of the present study but decreases its external validity. Specifically, the students may not be representative of chemistry students (e.g., with respect to interest in the material). Consequently, future research should examine whether the present findings generalize to chemistry students.

Further, although students had no prior exposure to energy diagrams, they had prior ideas about chemistry concepts, as discussed above. Therefore, it is impossible to conclude that the study materials caused the observed challenges but merely that they arose in the context of students' exposure to energy diagrams. Conceptual challenges are likely caused by a complex set of factors that include prior knowledge as well as the present instructional materials.

Finally, the present study qualitatively examined students' conceptual challenges. Gathering additional quantitative data, for example using a validated instrument like the QuPRI concept inventory,[35] would allow connecting the present findings with reliable measures of students' understanding of concepts depicted by AOEDs.

CONCLUSIONS

The present study documented conceptual challenges that arise among naïve students in the context of AOEDs. The study focused particularly on students' understanding of arrows that denote electrons, which is a visual feature shared across many types of energy diagrams. While AOEDs are prevalent in chemistry education, they are an under-researched type of visual representation. Our study indicates that AOEDs contain visual features that are confusing to students, thereby taking a first step toward helping instructors address conceptual challenges with AOEDs. The present findings can inform instructional practices not only with AOEDs but also with other types of energy diagrams that are visually similar to AOEDs.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.1c01135.

Additional demographic information (PDF)
Interview protocol (PDF)

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Notes

The authors declare no competing financial interest.

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