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Identifying Student Use of Ball-and-Stick Images versus Electrostatic Potential Map Images via Eye Tracking

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ABSTRACT: This pilot study examined students' use of ball-and-stick images versus electrostatic potential maps when asked questions about electron density, positive charge, proton attack, and hydroxide attack with six different molecules (two alcohols, two carboxylic acids, and two hydroxycarboxylic acids). Students' viewing of these dual images was measured by monitoring eye fixations of the students while they read and answered questions. Results showed that students spent significantly more time with the ball-and-stick image when asked questions about proton or hydroxide attack, but equal time on the images when asked about electron density or positive charge. When comparing accuracy and time spent on the images, students who spent more time on the ball-and-stick when asked about positive charge were less likely to be correct, while those who spent more time with the potential map were more likely to be correct. The paper serves to introduce readers to eye-tracker data and calls for replication with a larger subject pool and for the inclusion of eye tracking as a chemical education research tool.

KEYWORDS: *Molecular Modeling, First-Year Undergraduate/General, Chemical Education Research, Molecular Properties/Structure, Multimedia-Based Learning*

FEATURE: Chemical Education Research

■ BACKGROUND

Early on, the belief was that teaching chemistry phenomena algorithmically or mathematically promoted not only the understanding of problem solving, but also the understanding of the particulate nature of matter (PNM).[1] Even those with constructivist theoretical backgrounds held this belief. Constructivism includes the beliefs that: (i) knowledge is constructed from interactions with people and materials, not transmitted; (ii) prior knowledge impacts learning; (iii) learning, especially initial understanding, is context specific; and (iv) purposeful learning activities are required to facilitate the construction or modification of knowledge structures.[2−5]

Despite emphasis on mathematical algorithmic instruction, researchers found that misconceptions concerning the PNM existed for students at all levels from primary to graduate school.[6−8] Further, a gap was reported between students' ability to respond to algorithmic questions versus their lesser ability to respond to conceptual questions.[1,9,10] The shortfall in answering conceptual questions is at odds with the fact that chemists explain experimental results by theoretical explanations that usually involve particles or conceptual reasoning, giving rise to the expert-novice differences described by a number of researchers (e.g., ref 11).

Several researchers, including Johnstone,[12] proposed that chemistry has multiple representations: observable evidence (macroscopic); mathematical and chemical symbols (symbolic); and several different representations of atomic, molecular, and particle structure and behavior (submicroscopic or particulate). Johnstone's categories lead to the idea that the gap between algorithmic and conceptual understanding may stem from students' inability to translate effortlessly between these multiple representations, because often, conceptual questions deal with particle behavior, while algorithmic questions are mathematical in nature (symbolic). A number of studies have confirmed that students' misconceptions result from application of macroscopic explanations, those derived from their everyday experience, to particles,[13,14] or by students' inability to visualize, diagram, or depict the behavior of particles.[15,16] These studies give rise to the issue of how students visualize particle behavior or attributes.

Visualization can be defined as: (i) the creation of a clear picture of something in the mind; or (ii) a clear picture of something created in the mind.[17] What can chemistry instructors do to help students visualize or create a mental picture of particles? In their review of the literature, Williamson and Jose[18] found reports that particulate mental models could be simulated by using a number of techniques, including:

- Using physical models to represent particles
- Allowing student to role-play as particles
- Using computer images that could be viewed and rotated
- Using dynamic computer animations of particles during a process

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- Allowing students to generate their own drawings or animations
- Using interactive computer visualizations in which students controlled most of the variables

Findings for studies using animations of particle behavior show that:

- Animations can be short in duration, but when used consistently during instruction, result in significantly higher level of understanding.[19,20]
- Students can make connections between the levels of representation when particulate animations and demonstrations are used conjunctively.[19,21]
- Gender differences with the use of animations may exist.[22]

Research with the use of two representations has usually involved sequential use of two different types of representations. For example, Velázquez-Marcano et al.[23] found that both macroscopic videos of the laboratory phenomena and particulate animations were needed when students were asked to predict the outcome of opening a stopcock between two flasks containing fluids or a vacuum. The macroscopic videos alone did not evoke maximum performance perhaps owing to the tenacity of alternate conceptions. The animations alone did not evoke maximum performance; perhaps these were not enough to enable macroscopic mental models, leading to the finding that both types of visualizations are necessary for students to predict outcomes. Further, while both the video and animation were needed, there was no preferred order.

Williamson et al.[24] repeated the experiment, but examined the explanations students gave for the phenomena. In addition, they gave students a side-by-side view of the macroscopic video and particulate animations. Findings include these:

- Both videos and animations are needed for maximum particulate understanding of the phenomenon.
- Order does matter. Macroscopic followed by particulate leads to significantly better performance.
- Viewing a video and animation simultaneously confuses students about the particulate nature of what they are viewing, with more research needed on simultaneous views.

Researchers have also examined how students relate different representations at the submicroscopic level. Sanger and Badger[25] found that using electron density plots that had the molecules' electrostatic potentials mapped onto them ("elpot" maps, termed EPM in the present study) sequentially with animations in addition to the traditional physical models and demonstrations gave a significantly better conceptual understanding of molecular polarity and intermolecular forces. In their study with college chemistry students, the animation and elpot maps were not shown simultaneously on the screen. The authors concluded (ref 25, p 1414):

> *We believe that the instructional effectiveness of elpot maps lies in their ability to help students visualize positive, neutral, and negative atoms in a molecule by means of color.*

If such electrostatic potential maps can be of benefit, what would happen if students were given simultaneous images? Ball-and-stick images (B&S) are the most common molecular representation used in textbooks. Which image will students use when answering questions if given both B&S and EPM images? It might be expected that use of the EPMs would quickly allow students to answer questions concerning electron density and positive charge, because this is coded by color in the maps. This study focused on student integration of the B&S and the EPM representations. Specifically, we focused on which representation a student chooses when answering chemistry questions about electron density, positive charge, proton attack, and hydroxide attack. We grappled with the issue of how to determine which image students use when faced with these questions. We wanted to see whether a technology more commonly used in other domains might help with this issue.

Eye-tracking technology, used in cognitive psychology research, appeared to be a promising technology. While the use of eye trackers is relatively new to chemical education research, they have been long used in psychological studies of reading,[26] scene perception,[27] and comprehension of diagrams and graphs in other domains (e.g., refs 28 and 29). When looking at a diagram or any other visual stimulus, our eyes do not move smoothly across the stimulus. Instead our eye movements consist of phases during which the gaze position is relatively still, called *fixations*, and phases when the eyes are moving rapidly from one location to another, called *saccades*. Typical fixations last about 250−300 ms, and it is during these fixations that the visual system is taking in information from the environment. Saccades typically take less than 30 ms, and during a saccade, there is no intake of visual information from the environment (so that we are not aware of our eyes moving in this way).[26,27] Eye fixations can be interpreted as a measure of overt visual attention.[27] In one recent study using chemistry content, researchers found that eye fixations and verbalizations were highly correlated,[30] adding support to the interpretation that eye fixation data give a good indication of where a student's attention is centered. This paper reports data from a pilot study using eye-tracking technology and suggests directions for our research community.

■ RESEARCH QUESTIONS

Our specific questions included these three:

1. Where do students focus when simultaneously shown B&S and EPM representations of a molecule with no specific question to answer?
2. When given the two images, where do students focus when asked specific questions about the molecules?
3. Is there a relationship between accuracy in answering questions and fixation time on the B&S versus the EPM image?

■ METHODOLOGY

Participants

Students who were enrolled in the second quarter of a three-quarter organic chemistry class at a research university were recruited; 9 students volunteered. These students had all completed a year of general chemistry and one-quarter of organic chemistry; they had previously studied the chemistry concepts and molecule types involved in the study. While the textbook used in their course[31] contained EPM images, the instructor made no reference to them in lecture, in homework, or on examinations. The subject population was chosen, in part, because of the existence of EPMs in their textbook; hence, they were potentially acquainted with EPMs, as well as with the molecules used. (These molecules are described in the procedure section.) The volunteers' experiences in past chemistry courses were not investigated in this pilot study.

We do know that EPMs are prevalent in most general and organic textbooks,[32] but they are usually only integrated into a few chapters in general chemistry and much more widespread in organic chemistry. Additionally, EPMs show up in the end-of-chapter questions much less frequently[32] than simply being present in the chapters. The volunteers seemed to be a rough cross-section of students, not weighted toward either extreme. Volunteers received $10 for their time at the conclusion of the session. While this is a small number of students, it is consistent with other published eye-tracking studies, in which 9−11 subjects participated.[28,30] In addition, the subjects here were taking part in a pilot study, so we wanted small numbers.

Hardware

Eye movements were monitored with an SMI EyeLink head-mounted eye-tracking system, which sampled the position of participants' eyes every 4 ms, that is, at a rate of 250 Hz. Participants viewed images presented on a computer screen while resting their chin on a chin rest set 30 in. from the screen. The computer screen measured 15 in. horizontally, × 11.5 in. vertically. The monitor's screen resolution was set to 800 × 600 screen pixels, with a refresh rate of 75 Hz.

Images

Images used in this study were generated using Spartan software, 2005 version. EPMs were generated with 92% bounding surface, an isovalue of 0.04 $e^-/Å^3$, and an absolute scale of −35 to +175 kJ/mol. Use of an absolute scale and consistent isovalues is essential for consistent representation of EPMs. Colors coded on an absolute scale show red for more negative electrostatic potential (−35 kJ/mol) to blue for more positive electrostatic potential (+175 kJ/mol). At present, some textbooks use an absolute scale; the textbook used by the students in this study[31] presents maps with an absolute scale. B&S images were generated using default Spartan settings.

Procedure

Students took part in the study one at a time. Each student reported to the testing center. After they signed a consent form, the eye tracker was calibrated. Students were then given a brief introduction into the content of an EPM, including the meaning of the different colors and sample images of water and sodium chloride. The connection between EPM and B&S representations was illustrated with the example of water. Next, students were shown illustrations, each containing an EPM and a B&S image for the same molecule and were allowed to survey the molecules without any labels or questions. This was done for six different molecules (two alcohols, two carboxylic acids, and two hydroxycarboxylic acids: common, simple molecules for introductory organic classes), which were presented in a random order. For half of the molecules (one alcohol, one carboxylic acid, and one hydroxycarboxylic acid), the B&S image was on the left, as in Figure 1; for the other half, the B&S image was on the right. Thus, we controlled for any effect due to the order of the representations from left to right. All molecules contained either one or two functional groups and were small (≤5 carbons), straight-chain or branched hydrocarbons. Figure 1 shows an example. Students were allowed to survey each set of the dual images for the six molecules for 10 s. The images were static, and no text was on the screen.

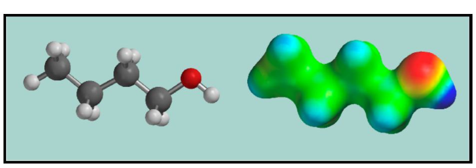

Figure 1. Ball-and-stick versus electrostatic potential map representations of 1-butanol.

Next students viewed the molecules while answering a total of 40 questions, which were presented in a random order. Four questions about each of the six molecules involved dual images. These 24 questions are reported here. The remaining 16 questions dealt with only one image and are not included in the analyses reported here. All four questions were asked for each of the six molecules (two alcohols, two carboxylic acids, and two hydroxycarboxylic acids). These four questions included:

Q1: Which atom in the molecule has the greatest positive charge?
Q2: Where would a proton attach in this molecule?
Q3: Where would hydroxide attack this molecule?
Q4: Which atom has the highest electron density?

The set of 24 questions were randomized to remove any effect of question order or molecule order.

Each question was accompanied by both representations of the molecule. The question was displayed on the screen, along with a unique question number for each question. Both the presentation of which representation was on the left side and the question order were randomized. Three atoms in each representation were also numbered by an experienced organic professor to disambiguate student references to particular atoms. These atoms were chosen as the correct answer (the most positive, the most negative where a proton would attach, the most positive where a hydroxide would attack, or the highest electron density), the opposite answer, or an atom that is between the correct answer and opposite answer. These were numbered in random order. Participants were notified that there was no time limit for this part of the study. The participants answered orally, and were required to answer by choosing one of the three numbered atoms as their answer. A research assistant noted their answers and the question numbers. See Figure 2 for an example.

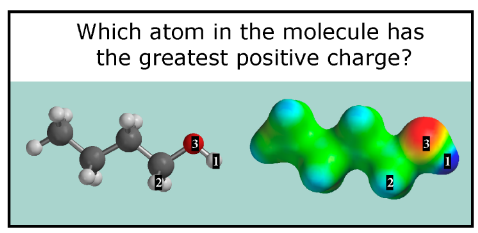

Figure 2. Question 1 with ball-and-stick versus electrostatic potential map representations of 1-butanol.

Data Coding

The eye-tracking data were first aggregated to detect saccades and fixations. The aggregation software was set to detect saccades with an amplitude of 0.05° or greater, an acceleration threshold of 9500° s^{-2}, and a velocity threshold of 30° s^{-1}, and fixations were defined as time between saccades. To analyze the locations of the eye fixations, we defined rectangular areas of interest on the display (see Figure 3) containing the B&S, the EPM, and the text, and analyzed both the number of fixations and the total amount of time spent fixating each region of interest, which we refer to as fixation time. (The number of fixations and fixation time were highly correlated, so we focused

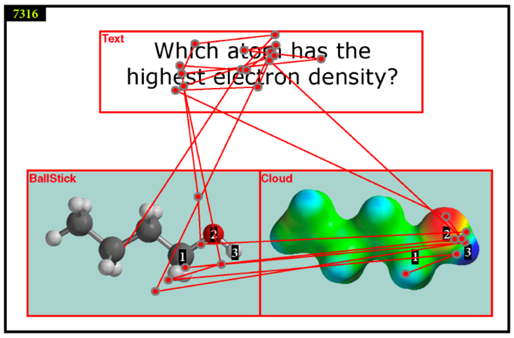

Figure 3. Example of a trial showing one student's sequence of eye fixations (consecutive eye fixations are linked by lines) and the rectangular areas of interest to which fixations were aggregated.

on fixation time in our analyses.) The two images were approximately 1° of visual angle apart and the eye tracker measures eye position to within 0.5° of visual angle, so it is unlikely that eye fixations were classified as in the wrong region of interest, especially given that eye fixations tended to be focused on a specific location within the images, depending on the question asked. (See Figure 3 for an example.)

■ RESULTS

On the 10 s survey of each pair of images, students spent an average of 8.15 s viewing one of the molecular representations. The remaining time was spent blinking, fixating white space, or reflected brief periods when calibration was lost. Table 1 shows

Table 1. Mean Fixation Time of Students Viewing the Images Displayed Alone[a]

	Mean Fixation Time, s (SD)		Significance[d]
Compounds	B&S[b] Images	EPM[c] Images	p-Values
Alcohols	4.5 (1.3)	3.5 (1.0)	0.26
Carboxylic Acids	4.2 (1.4)	3.8 (1.2)	0.59
Hydroxycarboxylic Acids	4.5 (1.3)	3.8 (1.4)	0.68
Overall	4.4 (1.1)	3.7 (1.0)	0.59

[a]Images were displayed alone, without any accompanying question text. [b]B&S: ball-and-stick representations. [c]EPM: electrostatic potential map representations. [d]Wilcoxon signed ranks test; $N = 9$.

the mean time spent fixating on the regions of interest corresponding to the EPM and B&S images for the three types of molecules and overall. While the trend was for participants to spend more time fixating on the B&S image than the EPM image, this difference was not statistically significant by a Wilcoxon Ranks test either overall or for any of the three types of molecules ($p > 0.25$ in all cases). Thus, the times spent on the two images were similar, and this pattern was evident for each of the three types of molecules.

The mean fixation time on the text, B&S representations, and EPM representations was calculated for each of the four questions asked with the six dual-image molecules. The mean fixation times are shown in Table 2 and in Figure 4, along with the total mean fixation time. For the positive charge and the electron density questions, no significant difference was found between the times spent on the B&S image and the EPM. The differences in the time spent between the B&S image and EPM were statistically significant only for Q2 and Q3, which dealt with proton and hydroxide attack. As Table 2 shows, these patterns were consistent across the three types of molecules in the problems (alcohols, carboxylic acids, and hydroxycarboxylic acids), with p values for the individual types of molecules either significant at the $p < 0.05$ level or at $p = 0.07$. For these attack questions, students spent significantly more time on the B&S image than they did on the EPM.

Accuracy was analyzed across the four questions. For each student, the maximum proportion correct was 1.00 for each question if it were correctly answered for all six molecules. Table 3 shows the mean proportion correct for each question based on the type of molecule and computed across all six molecules. Almost all participants correctly answered the questions on proton attack and electron density. The question on hydroxide attack was the least correctly answered question, with a mean of 0.55 (SD: 0.42), while the question on electron density had a mean proportion correct of 0.95 (SD: 0.08).

Correlations between accuracy (proportion correct for each question computed across the six molecules) and average time spent on either the B&S or EPM images for each question were computed (see Table 4). Across all four questions, the proportion of time on the B&S image was either negatively correlated with accuracy or had a zero correlation with accuracy, whereas the proportion of time on the EPM was positively correlated with accuracy for all questions. Thus, in general, students who were less successful in answering the questions spent more time focusing on the B&S images, whereas the more successful students used the EPM images. With our sample size, these likelihoods were not significant, as seen in Table 4.

■ DISCUSSION OF FINDINGS AND SUMMARY

It seems that students spend equal time with the B&S and EPM images when there are no questions posed. This suggests that there is nothing inherent in either of the images that draw the students' attention more than the other image. Equal student attention to the images without any text lends validity to the idea that fixations were due to prompts from the questions.

When questions are posed, results show that for questions on positive charge and on electron density, students looked equally at the B&S and EPM images. This is a little surprising to experts who would say that electron density and positive charge are more quickly determined by the EPM images. Perhaps the students were attempting to equate the two images. In contrast to questions on charge, when given the questions concerning proton or hydroxide attack, the students looked at the B&S image significantly more that the electrostatic potential map. Were the students simply defaulting to the more familiar image with these harder questions? Was there something inherent in the students that caused them to avoid EPMs?

Students had more difficulty answering the questions about hydroxide attack. Why was this more difficult than the proton attack questions? It seems that when the questions are more difficult (requiring additional knowledge or processing), students rely on the image with which they are more familiar, B&S representations. Questions that ask about hydroxide attack require that students know the charge of a hydroxide ion (negative) and that it will attack the more positively charged atom in the other molecule. Finally, students need to know that blue is associated with positive; therefore a hydroxide attack is at the blue location on the molecular representation. This requires several more steps than proton attack, because a proton is used interchangeably with a positive charge (taught early in a chemistry course). Students then simply have to say that the attack is at the negative location on the molecule,

Table 2. Mean Fixation Time of Students Viewing the Images and Text Together[a]

Questions and Molecules Shown	Mean Fixation Time for Each Component, s (SD)				Comparison of B&S and EPM
	Total	Text	B&S[b]	EPM[c]	p Value
Q1: Positive Charge (all 6 molecules)	6.9 (1.0)	1.8 (0.3)	2.2 (0.0)	2.5 (0.8)	0.26
Alcohols	6.2 (1.5)	2.0 (0.5)	1.9 (1.1)	1.8 (0.7)	0.95
Carboxylic Acids	7.3 (1.7)	1.8 (0.5)	2.4 (1.6)	2.4 (0.9)	0.95
Hydroxycarboxylic Acids	7.3 (1.3)	1.5 (0.3)	2.1 (0.6)	3.2 (1.3)	0.07
Q2: Proton Attack (all 6 molecules)	8.1 (2.7)	2.0 (0.3)	3.6[d] (1.4)	1.9[d] (1.3)	0.02[d]
Alcohols	6.9 (2.5)	2.0 (0.5)	3.1[d] (1.7)	1.5[d] (1.0)	0.01[d]
Carboxylic Acids	8.1 (3.4)	2.0 (0.7)	3.9[d] (2.3)	1.6[d] (1.1)	0.01[d]
Hydroxycarboxylic Acids	9.2 (5.1)	2.0 (0.6)	3.8 (1.6)	2.6 (2.4)	0.07
Q3: Hydroxide Attack (all 6 molecules)	10.0 (3.6)	2.2 (0.2)	4.6[d] (2.2)	2.6[d] (1.1)	0.01[d]
Alcohols	11.5 (7.6)	2.6 (1.5)	5.5[d] (4.6)	2.7[d] (1.7)	0.02[d]
Carboxylic Acids	7.9 (2.6)	1.6 (0.7)	3.5 (1.7)	2.2 (1.1)	0.07
Hydroxycarboxylic Acids	10.7 (3.1)	2.4 (1.2)	4.9[d] (2.1)	2.7[d] (1.1)	0.02[d]
Q4: Electron Density (all 6 molecules)	6.1 (1.8)	1.6 (0.4)	2.3 (1.1)	2.0 (0.6)	0.26
Alcohols	5.1 (1.6)	1.7 (0.6)	1.4 (0.5)	1.6 (0.6)	0.68
Carboxylic Acids	6.4 (2.4)	1.5 (0.3)	2.9 (2.1)	1.8 (0.7)	0.14
Hydroxycarboxylic Acids	6.9 (2.0)	1.4 (0.6)	2.4 (1.5)	2.6 (1.3)	0.68

[a]Images were displayed with the accompanying question. [b]B&S: ball-and-stick representations. [c]EPM: electropotential map representations. [d]Significant differences from Wilcoxon signed ranks test.

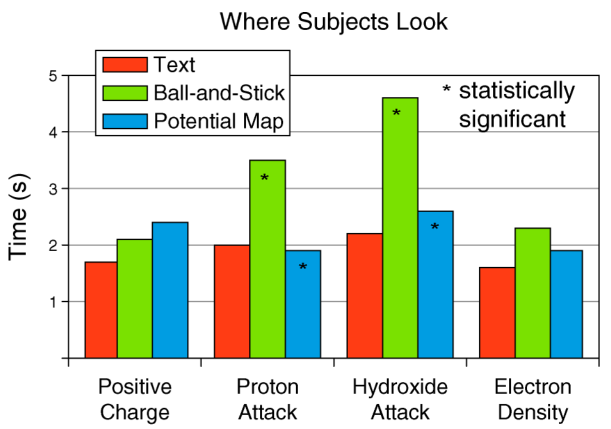

Figure 4. Mean fixation time with significant differences starred.

Table 4. Spearman Correlations Comparing Students' Accuracy and the Proportion of Time Spent on Images

Questions	B&S Images[a]		EPM Images[b]	
	Spearman Correlation	Significance[c]	Spearman Correlation	Significance[c]
Q1: Positive Charge	−0.475	0.196	0.337	0.337
Q2: Proton Attack	0.000	1.000	0.207	0.593
Q3: Hydroxide Attack	0.000	1.000	0.286	0.456
Q4: Electron Density	−0.311	0.416	0.414	0.268

[a]B&S: ball-and-stick representations. [b]EPM: electrostatic potential map representations. [c]Wilcoxon signed ranks test.

which looms large and red in both ESP and B&S images (an artifact of chemists using red for oxygen).

The relationship between accuracy and the time spent on an image was interesting, although our small sample size yielded no significant results when considering all six molecules. It was particularly interesting that for the positive charge and electron density questions there were negative correlations between accuracy and time with the B&S image: the more time the student spent with the B&S image, the more likely the student gave an incorrect answer. The correlation was zero for both of the attack questions. For all questions, positive correlations were found between accuracy and the time spent with the EPM image: the more time the student spent with the EPM, the more likely there was a correct response. Does more time on the EPM image indicate a more sophisticated view of molecules?

This pilot study using an eye-tracker demonstrates that eye tracking is an effective technology to probe use of multiple representations for answering particulate-level questions. Specifically, in this study it seems that students used the B&S image more when answering the harder, attack questions, but more successful students spent more time using the EPM image.

■ NEW DIRECTIONS

Further study with a larger sample is needed to test validity of these results across student differences such as reasoning ability,

Table 3. Distribution of Students' Correct Responses for Questions 1−4

Questions	Proportion of Students' Correct Responses by Molecule Type, Mean (SD)			
	Alcohols	Carboxylic Acids	Hydroxycarboxylic Acids	Average (All 6 Molecules)
Q1: Positive Charge	0.80 (0.41)	0.85 (0.37)	0.75 (0.44)	0.80 (0.33)
Q2: Proton Attack	0.95 (0.22)	0.95 (0.22)	0.80 (0.41)	0.92 (0.14)
Q3: Hydroxide Attack	0.65 (0.49)	0.55 (0.51)	0.47 (0.51)	0.55 (0.42)
Q4: Electron Density	1.00 (0.00)	0.95 (0.22)	1.00 (0.00)	0.95 (0.08)

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spatial ability, gender, previous chemistry knowledge, accuracy, and so forth. The study also needs to be done with general chemistry students. It should be noted that the eye-fixation data does not provide information about *why* students are looking at a particular image or *how* they are using the image to answer questions; instead these data tell us *if* they are looking at a particular representation. Can we ask probing questions to get students to spend more time with the images or a particular image? How do students' answers change with more directed questions? The eye tracker can be a tool to help with chemical education research, especially when images are involved.

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Notes

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