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Using Augmented Reality as a Tool for Distance Learning of VSEPR Theory

A Thesis Presented

by

Isabelle Lopez

To Keck Science Department

Of Claremont McKenna, Pitzer College, and Scripps Colleges

In partial fulfillment of

The degree of Bachelor of Arts

Senior Thesis in Molecular Biology

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Thank you to my family for the strength and patience they have given me throughout my undergraduate years. No podría ser la científica que soy sin el apoyo de ustedes. Todo lo que soy es gracias a ustedes.

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Abstract

Distance learning poses challenges in most academic settings, especially at the undergraduate laboratory level. Improving this mode of learning diminishes the impact of current events on young scientists' development of foundational laboratory concepts. Our work explores the use of augmented reality (AR) in a laboratory setting. We developed a completely virtual valence shell electron pair repulsion (VSEPR) theory lab activity consistent with the goals of Keck Science Department's Introduction to Chemistry course's in-person VSEPR lab activity. We were able to maintain a hands-on learning experience for students while using a tool many students already own: an iPhone as an alternative to model kits typically used for this lesson. Evaluating the efficacy of the AR lab activity was done in the Fall 2020 semester with Keck Science Department's CHEM14 class. I used a series of post-lab surveys, for instructors and students, to determine the efficacy of our approach and gauge students' experience with the technology. Ultimately, instructors and students found the lab activity helpful and felt AR was the most helpful in mastering VSEPR theory.

Introduction

The art of effectively teaching molecular geometry has long been a topic of interest among educators¹⁻⁵. At the undergraduate level, a strong conceptual understanding of the three-dimensional shapes assumed by molecules is foundational to students' chemistry education. Often taught in introduction to chemistry courses, mastering this concept paves the way for students' success in future chemistry courses such as organic chemistry, biochemistry, and more.

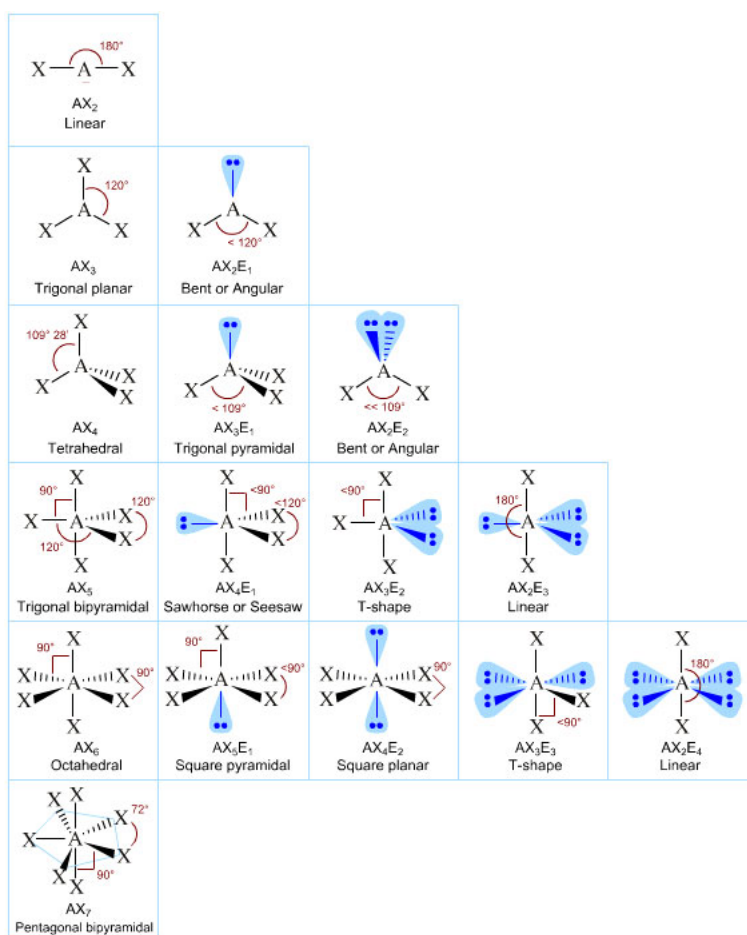


Figure 1. Chart of AXE system used to predict molecular geometries.

Valence shell electron pair repulsion (VSEPR) theory is the empirical model primarily used in predicting molecular geometries⁶. The theory allows stereochemistry to be predicted

based on the repulsive forces between electrons within the valence shell of an atom. VSEPR builds upon Lewis structures, where electron pairs are identified and their arrangement around a central molecule can be predicted to minimize repulsion. To determine what shape is assumed, molecules' make up can be translated into AX_nE_m , where A is the central atom, X is ligand, and E is the number of electron pairs⁷. For example, with a molecule like H_2O , the central atom (oxygen) has two ligands (two hydrogens) and two electron pairs, yielding a AX_2E_2 molecule with a bent geometry. Referencing the various AX_nE_m molecules, such as the those seen in Figure 1, this molecular make up produces a bent molecular geometry⁸.

The stereochemistry assumed as a result introduces geometries able to be visualized in three-dimensions (3D). While this 3D representation most accurately conveys the chemistry taking place, teaching this multi-dimensional representation has the potential to be challenging for some students. While many students can understand chemistry at the sensory level, visualizing and understanding symbols can sometimes be strained by a student's own daily experiences and exposure to conceptualizing 3D structures⁹. Thus, at chemistry's introductory level, it is critical that such experiences be considered by educators when teaching VSEPR theory and molecular structures. Such considerations ensure the classroom is an inclusive, effective space with the potential to positively influence students' learning experiences.

There are many mediums through which educators have approached teaching VSEPR theory. Many of these include engaging with tangible materials in lecture or laboratory to build the molecular shapes assumed by molecules. These materials include clay models, magnets, and even using a hand-held printer to produce two dimensional templates which can be constructed into 3D VSEPR shapes¹⁰⁻¹¹. A common visualization tool is the ball and stick model (Figure 2)¹². While many of these techniques have proven conducive to students' understanding of VSEPR theory, such approaches require physical materials to be used by all students.

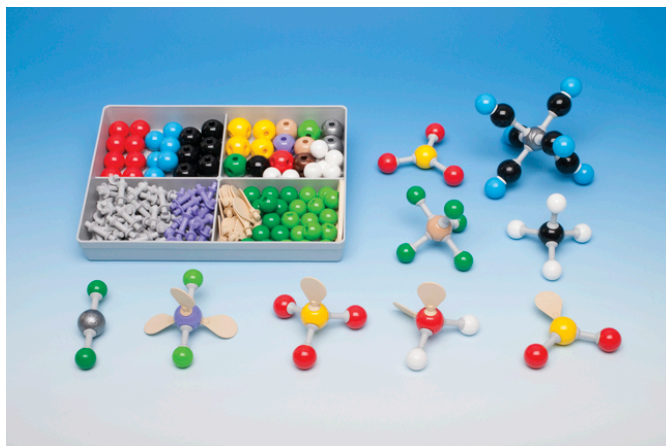


Figure 2. Ball and stick model kit typically used to teach VSEPR theory.

The threat of COVID-19 has introduced new public health guidelines in varying counties. At the national level, many schools and universities have shifted to distance learning to adhere to local health guidelines and ensure the health and safety of students, faculty, and campus staff (CDC). While applications like Zoom serve as an apt approach to lectures, it lacks the hands-on experience a student might engage with in a laboratory. Chemistry laboratories present to students the opportunity to learn laboratory skills and witness chemistry before their eyes. This level of interaction is difficult to replicate virtually. In fact, an entire issue of ACS's Journal of Education was dedicated to teaching chemistry during COVID-19. The inherent nature of Zoom eliminates students' ability to engage in traditional laboratory learning, especially of VSEPR theory. Relying on students to access 3D printing pens, clay, or model kits ignores students financial and home situations. Additionally, for science departments to purchase and ship such materials for all introduction to chemistry students poses challenges on the fronts of privacy and finances. Thus, current events pose a threat to students' conceptual understanding of the 3D structures in VSEPR theory.

Excitingly, another tool which has shown positive engagement from students is Augmented Reality (AR). AR imposes digital information on images in the physical world¹³.

The computer-generated elements are introduced to the real-world environment, visible to users via their device screen.

AR contrasts other mediums used to visualize 3D representations, including virtual reality (VR) and viewpoint manipulation (Figure 3)¹⁴. With Virtual reality, users wear a headset that allows users to be immersed in a computer-generated environment. The headset works to eliminate the outside environment, allowing users to focus on the 3D visuals and alter their gaze relative to the object to assume more visual information. Alternatively, viewpoint manipulation provides 3D visualization via a screen. Users may use hand-swipe motions to move the object and alter the object's spatial position in a way to best serve the user's critical understanding of the visual representation.

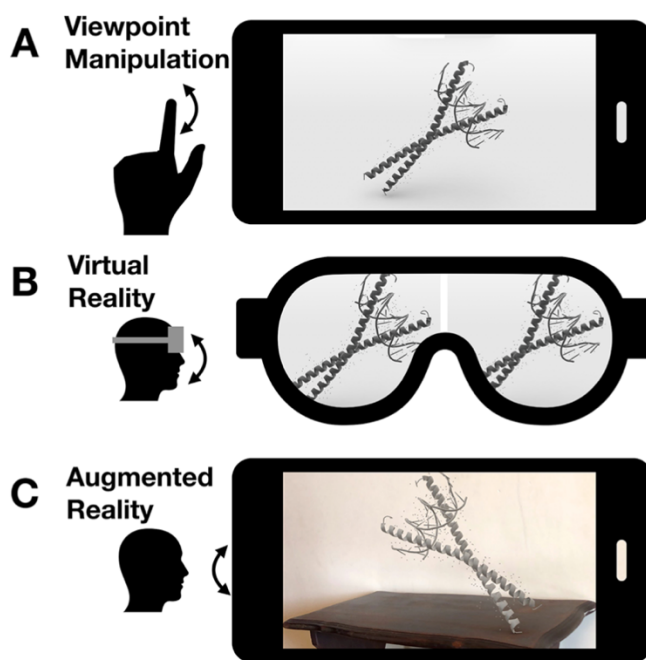


Figure 3. Schematic of visualization tools in viewing 3D information. 3D object is a “crystal structure of C/EBPbeta Bzip homodimer V285A mutant bound to a high affinity DNA fragment.” This figure was created by B. Sanii and used with permission.

The nature of these modes of visualization poise them as potentially useful tools for understanding 3D structures in the classroom. Virtual reality has been seen to be helpful in improving undergraduate chemistry students', particularly those with weaker spatial ability, understanding of the 3D nature of molecules. Viewpoint manipulation is also offered in chemistry labs, but limits students' understanding to interacting with a 2D screen to gain 3D information. However, VR limits the classroom experience, as students are required to put on a headset, eliminating the physical world to be immersed in a computer generated one. Viewpoint manipulation requires students to focus on their device screen, again limiting students' in-class engagement. Alternatively, augmented reality maintains an in-person environment, incorporating digital information into a user's physical classroom experience. Additionally, the materials necessary to incorporate augmented reality into the classroom are few. As mentioned, many students already have access to smartphone devices capable of engaging in AR visualization. Additionally, quick response (QR) codes have been leveraged to provide easy access to augmented reality tools within phones.

Existing work investigating the efficacy of augmented reality in chemistry laboratories suggests this tool may be helpful in different academic settings, including chemistry at the collegiate level ^{15,14}. Educators have found using AR useful in providing students with safety information and even to carry out in-lab titrations without chemicals ¹⁶. Beyond this, work has even been seen in the biochemistry classroom ¹⁷. In biochemistry, the chemical basis of structure and function of biomolecules, such as carbohydrates, lipids, proteins, and nucleic acids, is critical. Yet, visualizing these models can be challenging for some students. AR was shown to enhance students' understanding of protein visualization at the upper-division biochemistry level.

Mitigating visualization challenges requires leveraging materials students already have to learn VSEPR theory and other chemical concepts. With this in mind, a survey looking at ownership of iPhones among teens suggests 83% of teens have an iPhone¹⁸. Additionally, a survey done in 2019 with Keck Science Department students in an introduction to chemistry course indicated 83% of students regularly bring an apple device to class. Professors recently surveyed the incoming Fall 2020 Chem14 class on access to an iOS device and 91% of students reported to have access to at least one iOS device in their current living situation. Thus, it is reasonable to assume most students can access an apple device from home, presenting phones as a potential tool for distance learning.

Introducing new technologies into a curriculum is often challenging. These challenges include issues of accessibility to devices contributing to feelings of exclusion in the classroom. Other issues may include access to Wi-Fi and data plans. However, these issues may be accommodated by encouraging students to work in pairs, ensuring all students have at least one group member able to carry out AR functions.

Due to the Covid-19 pandemic, the Claremont College Consortium decided to do a virtual semester. The decision was made after much deliberation, but ultimately an in-person school year was deemed unsafe per L.A. County Department of Public Health guidelines¹⁹. This raised concern about ways to approach the laboratory activities with the incoming Introduction to Chemistry (CHEM14) class. Typically, in the fall, students learn foundational chemistry concepts such as stoichiometry, balancing equations, quantum, and VSEPR theory. In particular, students learn VSEPR via a lab activity where they are given a series of molecules and asked to use a model kit to create models and draw out their molecules. This lab activity often serves as excellent preparation for an exam and sometimes serves as preparation for an event known as a

“Dot-Off,” where students across introduction to chemistry course sections compete to create Lewis dot structures for given molecules.

The virtual nature of the fall semester put this lab in jeopardy. With these considerations in mind, myself and my labmates pursued AR as a means of supporting students’ multi-dimensional understanding of chemical concepts, especially VSEPR theory. To accomplish this, our lab created three dimensional molecules using various open-source platforms. We also incorporated viewpoint manipulation via a website, MolView, to show students key differences in electron geometry and molecular geometry. The worksheet was divided into various key concepts (polarity, lone pairs, isomers, and resonance), with molecules designated according to how well they might support students’ understanding of the concepts. We concluded the worksheet by presenting a key aspect of biomolecules, a peptide bond. Students were asked to visualize the peptide bond using AR and to use molecular geometry and resonance to explain the lack of rotation in a peptide bond.

In an effort to gauge the efficacy of this lab, a post-survey was done with students, teacher assistants (TA’s), and lab instructors. From the post-survey completed by the students, I hoped to understand students’ experience with the AR technology and to gauge what visualization tool best supported their understanding of VSEPR theory. From the post-survey completed by the TA’s and lab instructors, I hoped to learn how facilitators of the lab activity felt about the students’ experience with the AR technology and what visualization tool they thought best supported students’ understanding of VSEPR theory.

The implications of this study could suggest the use of iOS devices and AR serve as a potential tool for distance learning at varying levels of education, high school and collegiate. This would allow students, potentially at a national level, to engage with chemistry concepts remotely, using devices already readily available to them.

Methods

I. Producing 3D objects

To produce 3D objects, we developed a pipeline of software that would allow us to create desired molecules in line with correct geometric angles and color, according to common CPK rule ²⁰.

To create lone pairs, typically represented by a cloud with the unpaired electrons “inside,” we rendered a 3D rounded conical shape (Figure 4). The shape was made using the open-source software, OpenSCAD ²¹. OpenSCAD is a free software which makes solid 3D computer aided design (CAD) models out of script files. OpenSCAD is often used in creating machine parts to be printed by a 3D printer. These script files allow users to have full control over the exact shape taken by the model. We created a script that allowed us to produce lone pairs to be used in molecules that contained unpaired electrons (see Appendix).

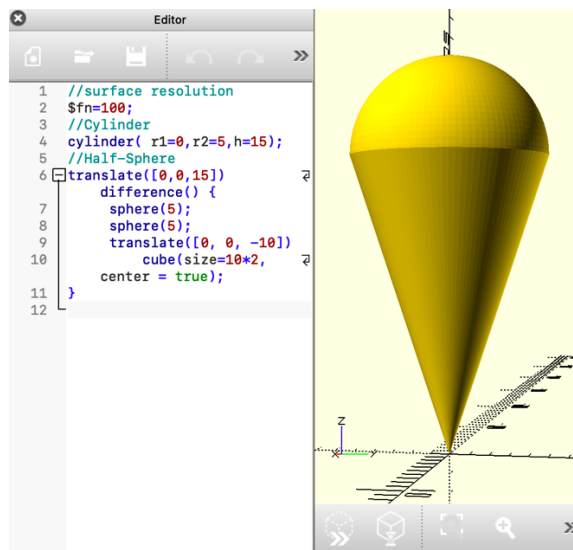


Figure 4. OpenSCAD script and the resulting design. Design be used to represent lone electron pairs.

To construct molecules, we used another free and open-source software, Blender ²². Blender allows for modeling, animation, simulation, and more, and it is often used in video editing and game design (Figure 5). This application encompasses an entire pipeline for

modeling creation, allowing it to serve as a major tool in many creator's development processes. Through blender, we were able to construct bonds using cylinders. This was accomplished by selecting Add > Mesh > Cylinder. The cylinder parameters could be altered by adjusting the scale on the X, Y, and Z axis. Its location and rotation relative to the origin could also be transformed along each axis. This allowed placement of objects relative to one another to be accurate with regard to angle and scale. The produced model was then exported as an .obj file.

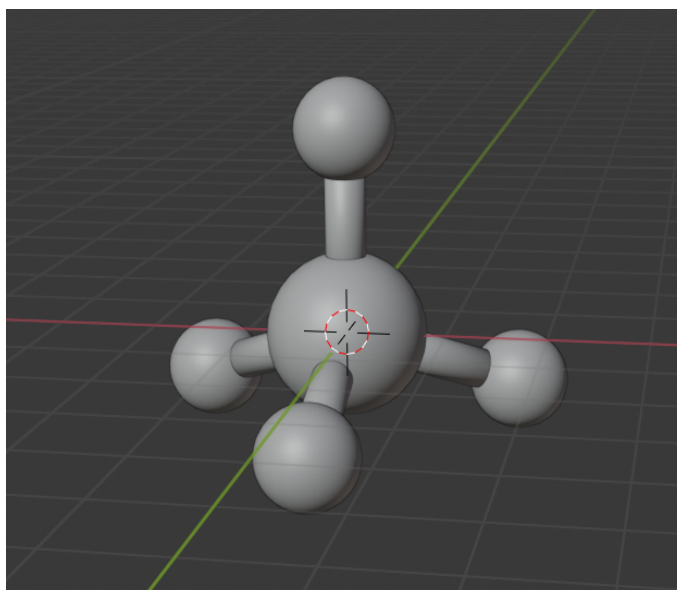


Figure 5. Blender editing interface. Here a simple tetrahedral is being produced.

The .obj files of the molecules were then uploaded to Xcode , a Universal app offered by Apple for app editing, to be colored and materialized ²³. In Xcode, the .obj file was visually provided, and selecting different components of the object permits edits (Figure 6). Such edits could be material (i.e. metallic, transparent), which transformed the way the object interacts with light, and slightly altered the look of the object based on where the view was relative to it. While in editing mode, one could add colors to the selected object piece as well. Once coloring the various parts of the molecule was done, the overall molecule was exported, again as an .obj file.

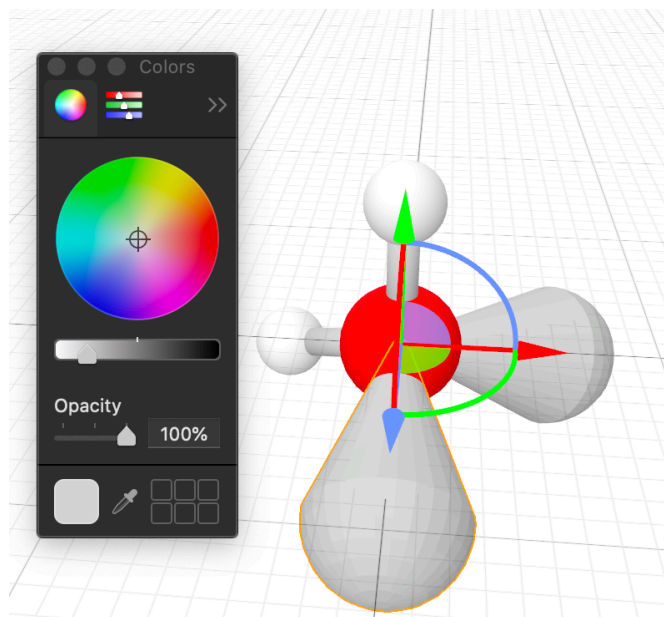


Figure 6. Xcode editing interface. Here a H₂O molecule is being colored. The red indicates the oxygen, and the white indicates hydrogen. The lone pairs depicted with the openSCAD design rounded-cone design.

The newly colored 3D molecule was converted into a file type viewable by AR on iOS devices using Reality Converter to convert the .obj file to a .USDZ file. Reality Converter is a free application available on iOS devices which allows users to convert, view, or customize USDZ objects. To carry this out, we were prompted upon opening the application to “Drop file here.” After carrying this out, we were able to see the object and manipulate our view of it by selecting the object with our mouse and swiping towards our desired vantage point.

To produce a QR code, the .USDZ files were uploaded to a file directory to produce a link to a file. This link was uploaded to a website which produced a QR code, in this case we used QR Code Generator²⁴. The QR code was chosen to provide quick access to the AR technology to students.

II. Creating VSEPR Worksheet

In producing the worksheet, our team first determined the common key goals educators typically strive for in teaching VSEPR theory. We referenced the VSEPR theory worksheet used

by the Keck Science Department in the past in an effort to ensure our approach was in line with KSD's past learning objectives.

The identified key concepts were: Polarity, Lone Pairs, Isomers, and Resonance. After determining these, molecules and/or sets of molecules were chosen for each key concept based on the degree to which the molecules supported conceptualization of the concept. Additionally, to encourage students to reflect on the key concepts and the examples, students "Check In" questions were incorporated in the worksheet. The Check In questions were provided with the intention of asking students to engage with the concepts and molecules on a deeper level.

It is important to note that the worksheet was completed by all students via Google Documents. This platform was decided on to minimize potential technological difficulties. Requiring students to print worksheets may have left some students feeling stressed or excluded if they have suboptimal access to a printer. Additionally, a non-virtual worksheet introduced a potential financial burden of printing the worksheet elsewhere. To avoid this, students were asked to complete the worksheet online.

Accurately producing Lewis dot structures is a fundamental first step in visualizing a molecule's 3D structure. This 2D representation of the molecule serves as a reliable guide to students when asked to visualize a structure in 3D. To do this, students were given a molecular formula and asked to produce a Lewis dot structure. A website which allows students to construct a Lewis dot structure was provided to students. We directed students to use St. Olaf College's Chemistry Toolkit. Using this site, students create a Lewis structure, screenshot their work, and paste the structure on the worksheet in a designated location.

Students were then asked to produce the molecular model to determine the geometry of the molecule using MolView. MolView is a website that allows users to construct a 2D structure, which it then renders to a 2D structure which can be viewed using viewpoint manipulation.

III. Producing and Dispersing Survey

To assess the efficacy of our approach, we produced a post-lab survey for instructors, teaching assistants (TA's), and students. The survey questions and distribution plan were approved by the Scripps Institutional Review Board (IRB). The survey was taken on Qualtrics. The link to the survey was provided to lab instructors/TAs via an email soliciting participation. Instructors/TAs were then asked to forward an email from myself soliciting participation from students.

Instructor/TA survey questions included:

1. Are you a lab instructor or a TA?
2. How helpful do you feel the lab activity was in supporting students' understanding of VSEPR theory?
3. How helpful do you feel augmented reality was in supporting students' understanding of VSEPR theory?
4. Do you feel augmented reality was helpful enough to be used in future chemistry lessons?
5. Did you notice several students having issues with any specific portions of the lab activity?
6. What changes would you make to the lab activity to make it more helpful to students?

The goal of these questions was to determine how helpful the lab was in achieving the goals of the lab. The role of AR in conceptualizing VSEPR theory was then determined via question 2. The usefulness beyond these unique educational circumstances was explored in question 4, hopefully reflecting true sentiments toward the efficacy of the lab. Qualitative

questions were then asked of lab instructors and TA's. These were asked to hopefully provide future directions to the project, suggestions can be used in optimizing the lab activity.

Student survey questions included:

1. Have you completed the VSEPR lab?
2. How well do you feel you know VSEPR theory after completing the lab activity?
3. What tool best helped you visualize molecules? (1 = "most helpful," 3 = "least helpful")
4. How helpful was AR in your understanding of VSEPR theory?
5. For a molecule with a trigonal bipyramidal molecular geometry, how many atoms are in the same plane? For reference, in the above tetrahedral molecule, the chlorines (Cl) are in the same plane.
6. Are there any changes you would make to the lab activity that would support your understanding of VSEPR theory?

The goal of these questions was to determine how helpful the lab was as a whole and AR specifically in supporting students understanding of VSEPR theory. The helpfulness of AR relative to other modes of visualizations in understanding VSEPR theory was determined via question 3. The level to which AR supported the conceptualization of VSEPR theory was determined via question 4. A question to understand student's ability to apply and visualize VSEPR theory was determined in question 5. Qualitative questions gauging how students would improve the lab were asked in question 6. These were asked to hopefully provide future directions to the project, suggestions can be used in optimizing the lab activity.

Results

Through troubleshooting various software pathways, we were eventually able to produce a software pathway that would allow us to create standardized molecules (Figure 7).

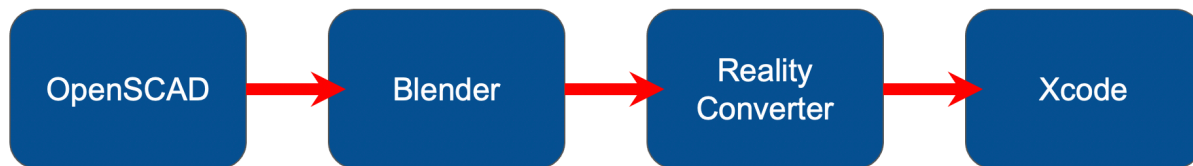


Figure 7. Final software pathway for creating VSEPR molecules

We used this plan to produce 20 molecules which we thought best exemplified key concepts of VSEPR theory. To support students' understanding of the influence polarity, H_2O and CO_2 were selected. To support students' understanding of lone pairs, NH_3 , NH_2^- were used to develop understanding the significance of type of electron group (lone pair or paired atom) on a molecule's geometry. To support students' understanding of isomers, PF_3Cl_2 was used because varied isomers may take on similar structures but adopt differing polarity. CH_2Cl_2 was also chosen to conceptualize isomers because of the molecule's two double bonds introducing a new level of complexity in understanding the relationship between slightly more complex molecules and geometry. To support students' understanding of resonance, NO_3^- and SCN^- were helpful in differentiating isomers and resonance in relation to geometry. To support students' understanding of complex molecular geometries, C_2H_4 , C_2H_6 , PF_5 , and SF_6 were chosen as effective in understanding the result of two central atoms on molecular geometrics as well as the varied complex structures adopted by elements capable of 'expanding' their octet. An application-based question was posed at the end of the worksheet. For this, students were asked to apply their gained knowledge of resonance and geometry to explain rotation about a peptide bond. Students were provided with an AR representation of the rigid unit to serve as support in thinking through the question.

These carefully chosen objects and examples were then organized into a worksheet for students to complete as a lab assignment. For each molecule, students were provided a formula. The students were then asked to indicate the correct VSEPR notation, produce and paste a Lewis Dot Structure, produce and paste the molecules molecular geometry and indicate its polarity, and scan and past the AR depiction of the molecule's electron pair geometry. All tasks were completable via Google Docs. An example of the worksheet set up can be seen in Figure 8.

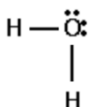
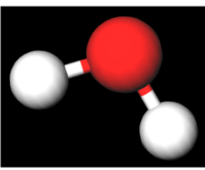

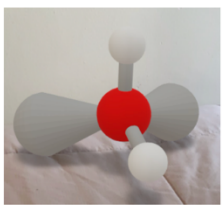
| Exploring Polarity! | | | |
|---|---|--|---|
| Formula | Lewis Dot Structure (include non-zero formal charges) | Molecular Geometry | Electron Pair Geometry (Paste your/your partners AR) |
| <p>1. H₂O</p> <p>VSEPR Notation: AX₂E₂</p> |  |  <p>Name: Bent Polar/Nonpolar (P/N): Polar</p> | <p>Scan:</p>   <p>Name: Tetrahedral</p> |

Figure 8. An example of a single question on the VSEPR worksheet using H₂O as a sample molecule. H₂O was used to illustrate the relationship between VSEPR determined geometry and molecular polarity.

After completing the lab, professors and TAs were asked to participate in the survey and also to forward my call for participation for the students. on their experience with the lab. Professors and/or TAs then forwarded my call for participation for complete a survey about their experience with the VSEPR lab activity to students.

I. Lab Instructor/ TA Post-Lab Survey

In surveying the lab instructors and TAs, a total of 5 participants volunteered their time to fill out the survey. From this, only 1 participant was a lab instructor, and the other four individuals were TA's.

In response to the first question: "How helpful do you feel the lab activity was in supporting students' understanding of VSEPR theory?" 100% of participants reported the lab activity was "Very helpful" (Figure 9a).

In response to the question "How helpful do you feel the AR was in supporting students' understanding VSEPR theory?" 80% of participants reported AR as "Very Helpful" while 20% of participants reported it was "Somewhat Helpful" (Figure 9b).

In response to the question "Do you think augmented reality was helpful enough to be used in future chemistry lessons?" 40% of participants answered, "Definitely Yes" while 60% of participants answered, "Probably Yes" (Figure 9c).

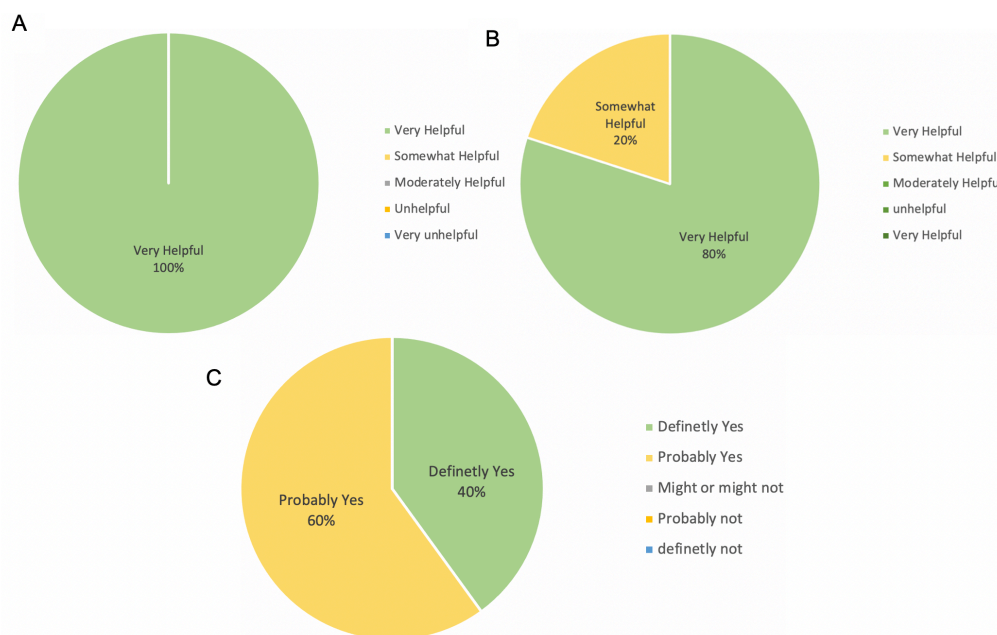


Figure 9. Lab Instructor and TA responses to survey questions (A) How helpful do you feel the lab activity was in supporting students' understanding of VSEPR theory? (B) How helpful do you feel the AR was in supporting students' understanding VSEPR theory? (C) Do you think augmented reality was helpful enough to be used in future chemistry lessons?

When surveying lab instructors and TA's "Did you notice several students having issues with any specific portions of the lab activity?" a few trends appeared in the written responses. With regard to technology, there was difficulty in loading "all of the images on their smartphones to take pictures with them." Additionally, one participant noted that "some people were having trouble with working the MolView." Some technological problem-solving is seen when one participant reported "[students] were easily able to screenshare on Zoom and help the 2 students in our section who didn't have iOS devices." Another participant noted "They were challenged by the very last question about the resonance of the bio-molecule, but I think that's actually a good thing."

Upon asking "What changes would you make to the lab activity to make it more helpful to students?" suggestions from participants varied. One participant suggested "providing part of a model kit would help them visualize better. The augmented reality was cool and helpful, but I think something tactile would help enforce the 3D concept just a little bit better." On a similar note, another respondent suggested "A combination of physical modeling kits and AR may be helpful to assist the different types of learners, but given the online environment, it may be challenging to provide physical kits." With regard to technology, one participant reported future work can be done in "trying to make it so that students who have do not have apple products can do the augmented reality part of the lab." Additionally, a participant noted "a simulation that shows lone pairs" would be great to supplement the worksheet.

II. Student Post-Lab Survey

In surveying the students, a total of 28 students volunteered their time to fill out the survey. In response to the first question "How well do you feel you know VSEPR theory after completing the lab activity?" 18% of participants reported to know VSEPR "A great deal" after completing the lab, while 50% of participants reported to know VSEPR theory "A lot," 29% "A

moderate amount,” and 3% “A little” (Figure 10a). No students reported not knowing VSEPR Theory at all.

In response to the question “What tool best helped you visualize molecules? (1 = “most helpful,” 3 = “least helpful”),” 53.8% of respondents ranked AR as “Most Helpful” in visualizing the molecules (Figure 10b). Alternatively, 42.3% of participants ranked MolView as “Helpful,” and 61.5% of participants ranked Lewis Dot Structures as “Least Helpful” in visualizing VSEPR molecules.

In response to the question “How helpful was AR in your understanding of VSEPR theory?” 43% of respondents reported AR as “Very Helpful,” while 21% found AR “Helpful,” 25% found AR “Somewhat Helpful,” and 11% of participants found AR “Not Helpful” in understanding VSEPR theory (Figure 10c).

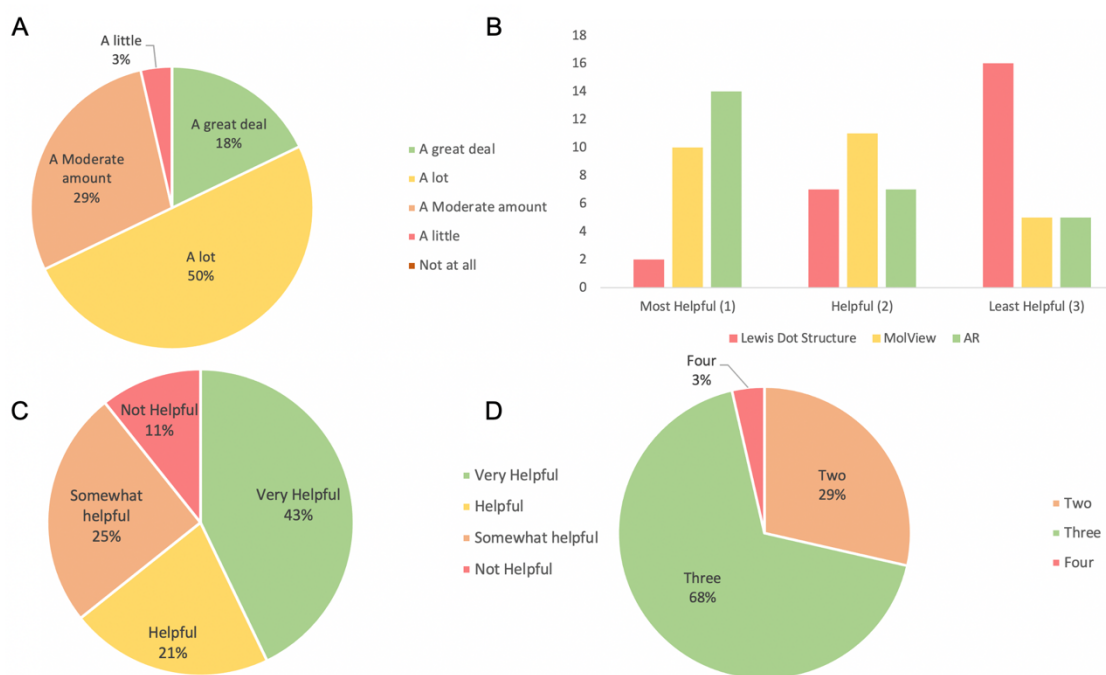


Figure 10. Student responses to survey questions (A) How well do you feel you know VSEPR theory after completing the lab activity? (B) What tool best helped you visualize molecules? (C) How helpful was AR in your understanding of VSEPR theory? (D) For a molecule with a trigonal bipyramidal molecular geometry, how many atoms are in the same plane?

In response to the survey question “For a molecule with a trigonal bipyramidal molecular geometry, how many atoms are in the same plane? For reference, in the above tetrahedral molecule, the chlorines (Cl) are in the same plane” the correct answer was three (Figure 10d). The tetrahedral provided can be seen in Figure 11²⁵. 68% of respondents accurately selected three, whereas 29% of students inaccurately answered two and 3% of students answered four.

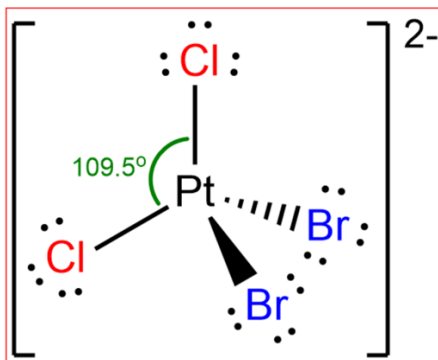


Figure 11. Example tetrahedral structure used to depict what “same plane” meant in question 5.

Upon asking participants if there “any changes you would make to the lab activity that would support your understanding of VSEPR theory?” some structural suggestions arose as well as suggestions regarding technology used. One included “I failed to see the connection between each category and why we did it. I would say have some sentences between each.” Another individual noted it would be helpful to have “clearer instructions...it was hard to understand what was needed to answer a question. This took some time away from understanding the content.” MolView specific comments included that “the MolView program was very frustrating” and “was difficult when making isomers because the orientation wasn’t what you would think it would be when it switched from 2D to 3D.” AR specific comments included “make the AR available for Android phones, too,” “the repulsion between the valence electrons causes different geometry,” and “AR was glitching at times, but overall it was helpful.”

Discussion

In an effort to determine how augmented reality may be used as a tool for distance learning of VSEPR theory, we were able to integrate a series of molecules' electron geometries into a lab activity for the Keck Science Department's CHEM14 lab. Producing an alternative mode of tools to learn VSEPR theory was considered pertinent as distance learning became necessary for schools worldwide. While previous approaches to learning VSEPR theory have included the use of a ball and stick model, research on the efficacy of augmented reality in facilitating students' understanding of 3D chemical and biochemical concepts in the classroom suggested AR might be a beneficial learning tool.

In addition to using AR, we were also able to incorporate other mediums of visual representation of VSEPR. Other visual tools we used included viewpoint manipulation for viewing molecular geometries and 2D information for viewing Lewis Dot structures. Students were able to engage with these tools to complete a VSEPR worksheet via Google Docs. The worksheet included concept checking questions which were meant to serve as a way for students to deepen their understanding of how VSEPR theory influences molecular geometries. After completing the lab activity, lab professors/TA's and students were asked to complete a post-lab survey on their experiences supporting students and completing the lab, respectively.

From the instructor/TA post-lab survey, it seems that all participants found the VSEPR lab to be very helpful in students' understanding of VSEPR theory. The level to which AR contributed to the helpfulness of the lab as a whole varied slightly, with 80% of participants reporting AR was "very helpful" and 20% of participants saying it was "somewhat helpful." In answering whether or not AR was helpful enough to be used in future chemistry lessons, some uncertainty appeared as 40% respondents answered, "Definitely Yes" and 60% of respondents answered, "Probably Yes." While this seems slightly inconsistent with the earlier question of the

degree to which AR was helpful, this deviation in confidence of the efficacy of AR in future chemistry lessons may be rooted in uncertainty towards students' perception of the technology. It is reasonable that answering this question definitively might be challenging for some participants without having directly speaking to students about their experience with the AR technology. Additionally, apprehension to answer definitively could be the result of wanting changes to be made to the technology before incorporating AR into chemistry activities again. Overall, the results suggest lab instructors and TA's perceived AR as helpful and would consider using it in future chemistry education settings.

Limitations of this survey must be emphasized in looking over the data. One limitation is that there were only five responses to the Lab Instructor/TA survey. Of these five, one was an instructor and 4 were TA's. These numbers make sense, as it may be challenging to volunteer to engage in more screen time than is already being asked of instructors and TA's. Additionally, it should be noted, as one respondent candidly reported, "students mostly did the lab on their own time...I didn't observe them doing the AR portion." The current organization of CHEM14 labs resemble that of a "flipped classroom." This consists of students doing a lab before their "lab time," and coming to their designated lab time with questions on the lab they were asked to finish. Under in-person circumstances, students are typically asked to complete a lab activity in the lab *during* their lab time, and lab instructors and TAs facilitate the lab by providing initial instruction, answering student questions, and ensure lab safety. This change in the chemistry lab structure may have limited instructors' and TAs' ability to engage with students and report on which aspects of the lab activity students found helpful or challenging. Additionally, if students had positive or negative experiences with aspects of the lab, some students may have sought support with peers or navigated a challenge themselves, and not spoken to an instructor. All these scenarios as well the number of participants should be factored in when reviewing the data.

From the student post-lab survey, it seems students' experience with the lab activity and the AR component varied but was generally positive. After completing the lab, most students had an improved understanding of VSEPR theory, with 18% reported they knew it "a great deal", 50% reported "a lot", and 29% of reported "a moderate amount." To evaluate which tool best helped assisted students in visualizing the molecules, participants were asked to rank tools from 1 being "most helpful," 2 being "helpful," and 3 being "least helpful." Overall, students seem to have found the AR the most helpful, followed by MolView and Lewis Dot structure, respectively. In determining exactly how helpful AR was, 42% participants reported it was "very helpful," 21% reported it was "helpful," 25% reported it was "somewhat helpful," and 11% reported it was "not helpful." These varying attitudes could be due to differing factors, including not having access to an iOS device and therefore not being able to visualize the molecules. In fact, one of the three students who answered, "not helpful" also suggested making "the AR available for Androids, too." The other two students had no suggestions. Additionally, some students reported the AR was "glitching at times, but overall helpful." A TA also reported students having trouble taking photos of the molecule on their phones, but this was not mentioned when surveying students on what changes they would make to the lab. All of these may have contributed to the varying student perspectives of the AR component of the lab.

Upon asking students to engage with 3D visualization in question 6, where students were asked to report how many atoms in a trigonal bipyramidal molecular geometry were in the same plane, 68% of students answered correctly. This suggests that 32% of students may have struggled in visualizing the molecule, forgotten the trigonal bipyramidal geometry, or were confused by how the question was worded. The later possibility could likely be plausible because the reference image provided to students to explain the idea of "in the same plane" may have

confused students. Overall, it appears most students found AR to be the most helpful in the lab activity and had a relatively positive experience.

Some limitations of the student post-lab survey should be considered when looking at the data. One limitation includes the number of student participants, which represent only 28 of the ~200 CHEM14 students. Additionally, many students completed the survey the Monday after their first exam and slightly over a week (depending on the time of students designated lab time) after having completed the lab. Thus, some details about the activity, including challenges and general experiences with the AR, might have been difficult to recall upon completing the survey. In answering the question about the number of atoms on the same plane, this information may have been fresher in the mind of students after having completed the survey directly after submitting their lab worksheet. Additionally, more questions in the survey could have been asked to determine what areas students struggled with most and why that might have been. A pre-lab assessment would also have been helpful in comparing students' perspectives towards AR before and after the lab activity.

Future work can be done to increase students' access to the AR technology. This may consist of creating a technology rent service via the science department for students. Additionally, making AR available through more devices would be very helpful, and should be investigated further. This may consist of converting .obj files into a file compatible with alternative smartphone AR file types. Aside from AR, it seems that students found MolView quite challenging at times. Thus, integrating an alternative system to depict molecular geometries might be helpful. Such systems could be an improved source to engage with viewpoint manipulation or providing students with AR models for molecular geometries as well. Another system, which connects with what was mentioned in the lab instructor/TA post-lab survey, is to supply students with tangible materials. While this is difficult with a late-notice, virtual semester,

it is unclear how effective AR is in supporting students' visualization of VSEPR theory relative to the traditional ball-and-stick model. A future study might include surveying students understanding of VSEPR theory after having done an AR VSEPR lab versus a ball-and-stick model VSEPR lab.

Overall, it seems that students and educators had a positive experience with AR, as well as the lab activity as a whole. Moving forward, with accessibility adjustments to technology in mind, it seems AR would be an apt approach to teaching three-dimensional concepts in the classroom. This may consist of building upon the current VSEPR lab by animating how bond angle changes as a result of electron repulsion. Beyond introduction to chemistry, AR technology may even be useful in the organic chemistry classroom. Having animation of a chair confirmation flip or SN2 versus SN1 reaction may be incredibly beneficial to students. Additionally, this lab activity incorporated AR visualization of augmented reality, which one instructor noted students found challenging, but that was a "good thing." Using AR to visualize more biomolecules in classes like biochemistry and molecular biology would might be supportive of students' understandings of biomolecules. Additionally, in molecular biology, animating more complex molecular mechanisms may assist students as well.

The applications of augmented reality bountiful and exemplify the many different ways educators can adapt their approach to teaching to best meet the needs of students. As our classrooms and technologies change, centering students' experience and gain from teaching tools is important more than ever in supporting the next generation of scientists.

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Appendix

OpenScad Lone Pair Script:

```
//surface resolution
$fn=100;
//Cylinder
cylinder( r1=0,r2=5,h=15);
//Half-Sphere
translate([0,0,15]) difference() {
  sphere(5);
  sphere(5);
  translate([0, 0, -10])
    cube(size=10*2, center = true);
}
```