MoleculAR Geometry: Chemical Visualizations in Augmented Reality

by

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Abstract

"MoleculAR Geometry" is an augmented reality (AR) application developed for the Magic Leap augmented reality headset. The application aims to serve as a learning aid for teaching 3D molecular configurations in general and organic chemistry laboratories and classrooms. The finished app includes eight types of molecular geometries along with examples and information on the number of bonds and lone electrons. A quiz game within the app assesses student understanding and sends results to the instructor. "MoleculAR Geometry" has undergone initial user testing at Middle Tennessee State University and is available on the Magic Leap devices in the James E. Walker Library.

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Introduction

Chemistry students historically struggle visualizing three-dimensional concepts such as molecular geometry (the 3D shape of a molecule) because of the disparity between the students' understanding of 2D depictions on paper and the 3D nature of the molecule (Johnstone, 1991). Although students typically understand how to draw 2D depictions of molecules, it is often difficult for students to pair the 2D structure with its 3D counterpart (Chandrasegaran & Treagust, 2008). This disparity is due to lack of students' spatial reasoning, a skill that is essential in order to succeed in chemistry (Harle & Towns, 2011; Oliver-Hoyo & Babilonia- Rosa, 2017). Instructors have attempted to combat this issue through the use of physical 3D models and computer visualizations (Sanger & Badger, 2001). However, one technology that has broad applications in 3D visualizations is augmented reality (AR), a technology that overlays virtual images on top of the real world. One of the most popular examples of this is the game Pokémon Go, a smartphone app that allows players to capture virtual Pokémon while walking around their physical environment. As AR innovations improve, many educators believe that chemistry classrooms and laboratories – not just video games – would benefit from augmented reality visualization aids (Maier & Klinker, 2013).

Students in the MTSU Chemistry Department, particularly in organic chemistry courses, regularly participate in computer-aided laboratory exercises that demonstrate concepts instructors are not able to demonstrate in a traditional laboratory setting. These exercises are typically completed using the molecular visualization software Spartan. Augmented reality would take this experience to a new level;

instead of viewing models on a computer screen, students would be able to view, manipulate, and walk around holographic molecules right in front of them. A supplemental lab in molecular geometry would be especially beneficial because molecular geometries form the foundation of concepts addressed in both general chemistry (freshman-level) and organic chemistry (sophomore-level) classes (Hornbuckle, Gobin, & Thurman, 2014; Bodner, 1986; Pribyl & Bodner, 1987).

When constructing an augmented reality application, the developer must consider several factors. First, she must decide which hardware to use and consider its limitations. One can develop augmented reality applications for a plethora of devices, including smartphones and mixed reality headsets. Smartphones are easily accessible and less expensive than headsets; however, their small screen size does not afford the illusion of being immersed in a virtual environment. For students to interact with models as if they were real, the developer should consider mixed reality headsets, which overlay images directly on top of the user's vision. One major headset available to developers is the Magic Leap, an augmented reality headset that uses a combination of glasses, computer pack (known as the "Lightpack"), and controller to place the user in an interactive environment. This project concerns the development of "MoleculAR Geometry," a Magic Leap application for chemistry laboratories that teaches the basics of molecular geometries.

Previous Work

Augmented reality has rapidly expanded into the gaming industry but has only touched the surface of education. The current educational AR applications are developed primarily for smartphones because of the devices' convenience and general availability among students.

Researchers at Middle Tennessee State University (MTSU) developed molecular visualization labs for organic chemistry for 3D computers and 3D glasses. However, there has not yet been any publicly available apps on the Magic Leap targeted specifically for education.

The progress that has been made in using AR for education shows positive preliminary results: students perform better on spatial reasoning tasks in AR as opposed to traditional teaching methods using 2D representations (Medicherla et al., 2010). In addition, AR has potential for helping students with learning or developmental disabilities. Students with ADHD have been shown to have increased attention span and motivation for learning when using educational AR resources (Chiazzese, G. et al., 2019). Additionally, AR technology is being used to help students with autism identify emotions and facial expressions as well as learn phonics and reading comprehension (Chen, et al., 2015, Howorth, et al. 2019). These preliminary results suggest that incorporating AR into classrooms will allow teachers to enhance learning across several student populations.

Summary of the Application

"MoleculAR Geometry" is compatible with the Magic Leap headset and features content relevant to general chemistry and organic chemistry classes and labs. This project differs from previous work done in the educational software development field because it utilizes an AR headset rather than 2D screens on phones or desktop computers. A headset lends the student a more immersive experience and allows for physical engagement with the lesson through the ability to walk around and interact with virtual content overlaid on top of the real world. The application was designed with a typical chemistry computer-based lab session in mind: students gather in a computer lab (or large room) and each receive a device then answer post-lab questions about the lesson content.

"MoleculAR Geometry" opens with an introduction scene, which introduces the student to eight different geometric orientations: tetrahedral, linear, bent, trigonal planar, trigonal pyramidal, trigonal bipyramidal, see-saw, and octahedral. The geometries, along with an example molecule for each, spawn radially around the user, forming a circular space in which the student can manipulate and read about several molecular shapes. A 2D representation of each molecule appears above its 3D counterpart, in addition to information panels that display the molecule name, geometry, number of electron pairs, number of bonds, and bond angles (see Figure 2). The student uses the Magic Leap controller as a virtual pointer by aiming it at a molecule. Once the student selects a molecule by pulling the controller trigger, he or she can move or rotate the molecule by holding down the trigger or swiping on the controller touchpad, respectively.

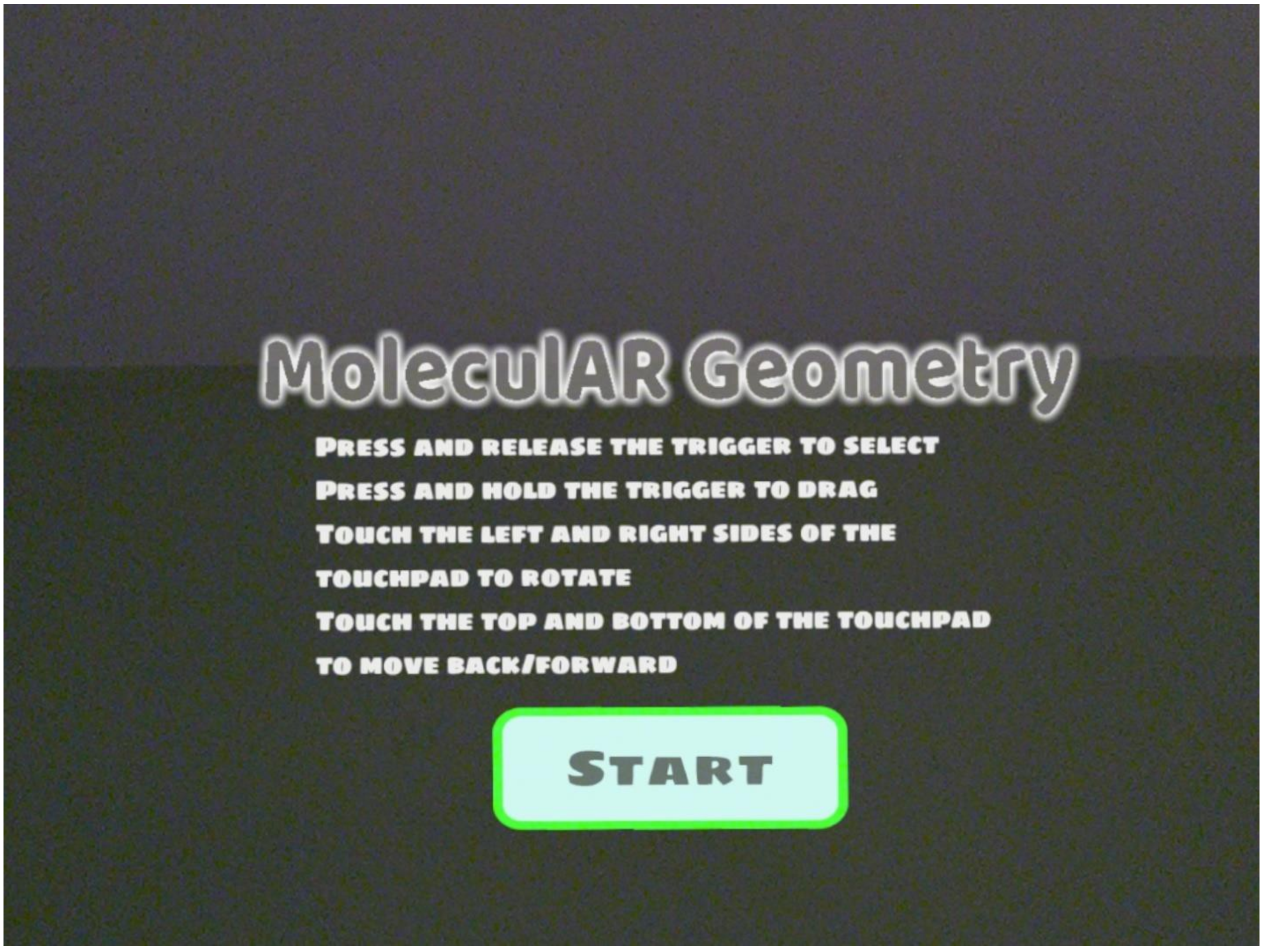

Figure 1. The opening menu of "MoleculAR Geometry," which explains the instructions.

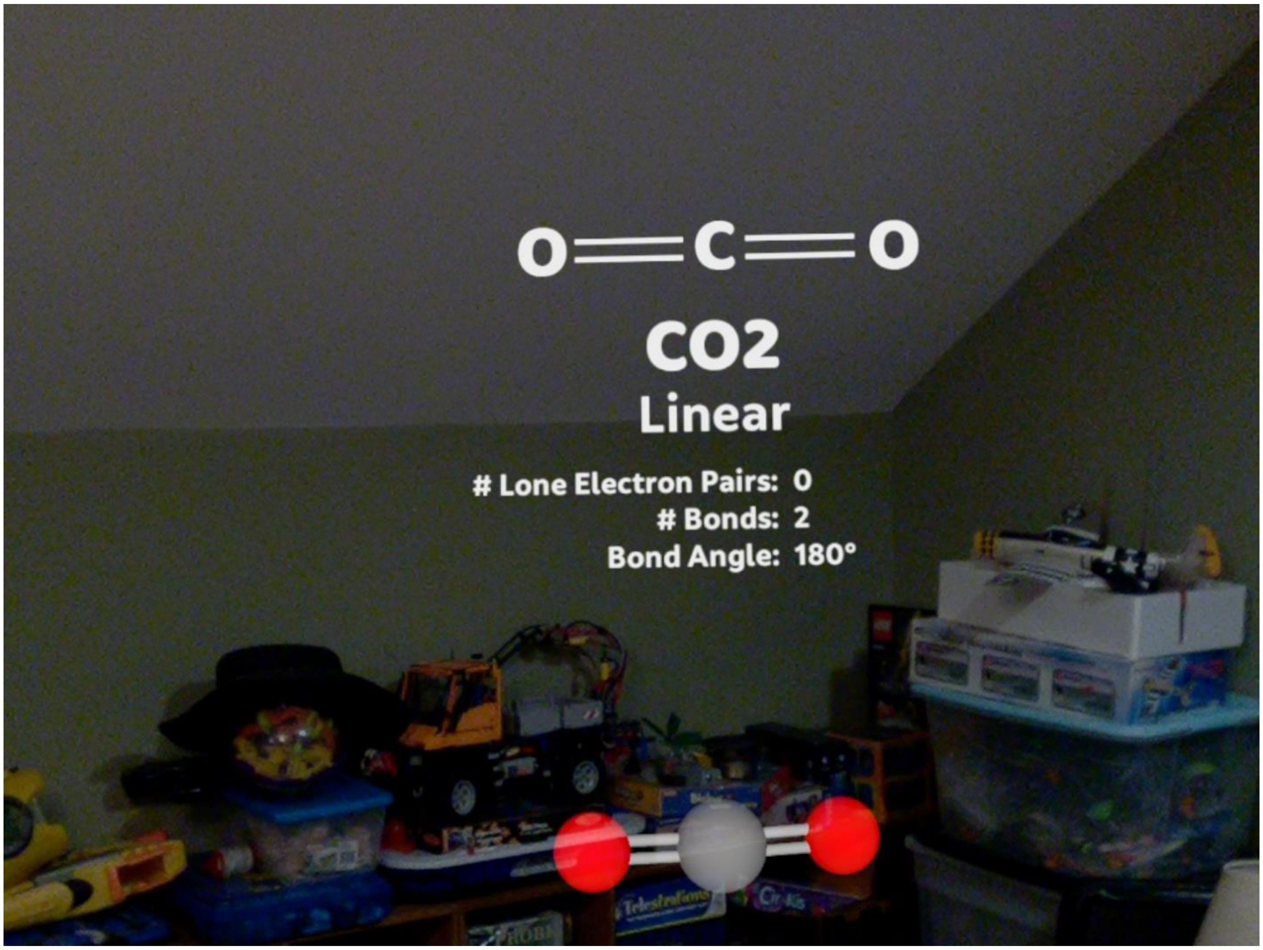

Figure 2. A screenshot from "MoleculAR Geometry." In this example, the user can see the 3D structure for carbon dioxide as well as its Lewis (2D) structure, geometry type, and bond information.

The user can access the main menu at any time by pressing the controller home button. From the menu, the user can choose to resume the application, continue to the app's quiz, read the app instructions, or view more options. The additional options include resetting molecule positions, placing the scene in a different location, or displaying geometric outlines or electron pairs.

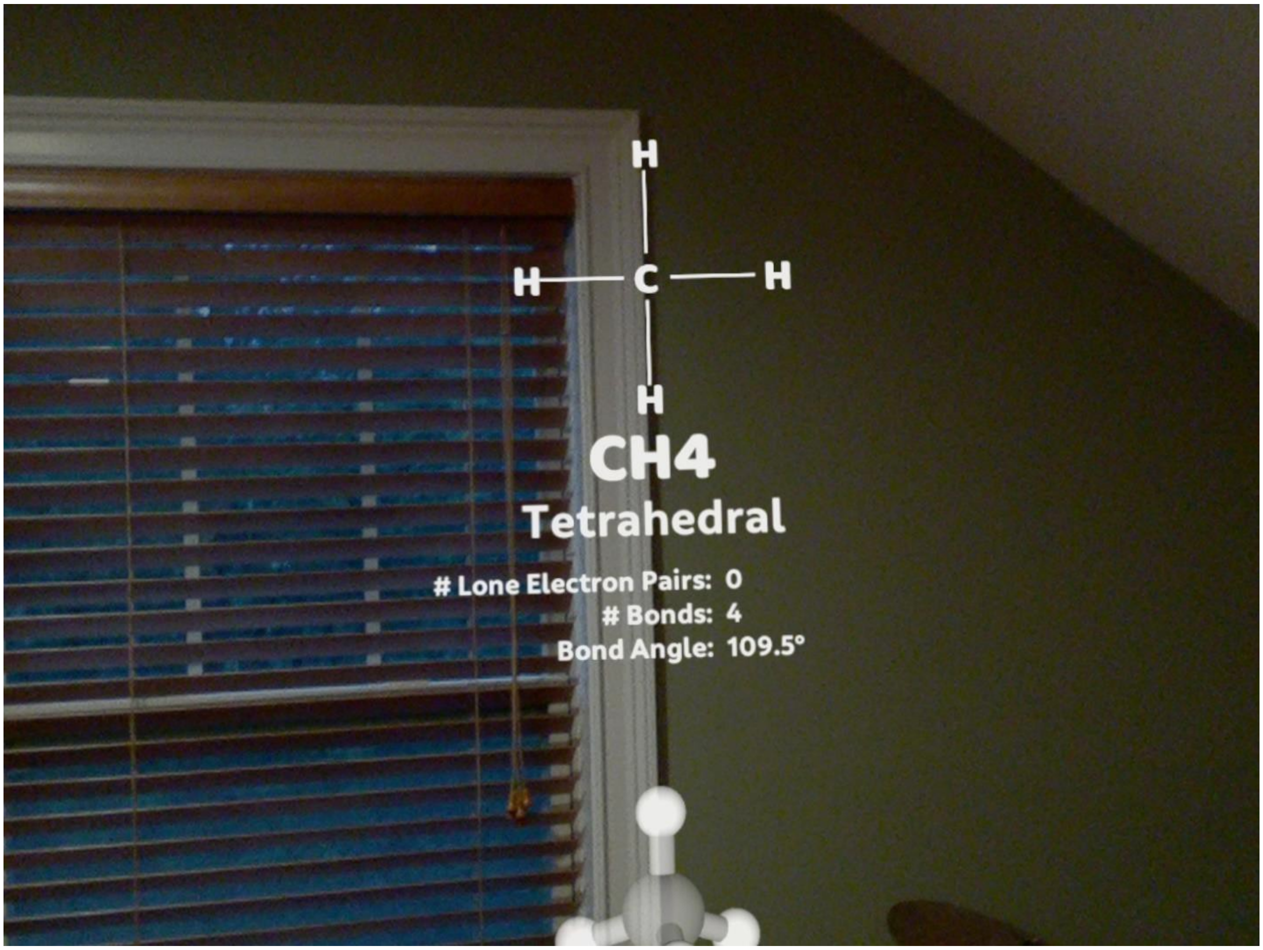

Figure 3. A screenshot of "MoleculAR Geometry" displaying information about methane. The 3D structure appears below.

After the student has finished exploring the introduction scene, he or she can select the “Go to Quiz” option from the main menu. In this scene, the labels of the molecular geometries are again placed radially around the user; however, there are no accompanying models or information. A virtual box appears in front of the user labelled with a 2D drawing of the molecule supposedly inside the box. The student must use the knowledge learned in the previous section, apply it to the new 2D molecule, and place the molecule in the correct geometric category (see Figure 4). Once the student places the box under the correct label, a 3D model of the molecule floats out of the box, and the user is free to inspect it. The student can then select a "Next Question" button, which causes a box labelled with a new molecule to appear. This process continues until the student answers all ten questions. At the end of the quiz sequence, the program displays the student's score and sends the results to a Google spreadsheet for the teacher to review.

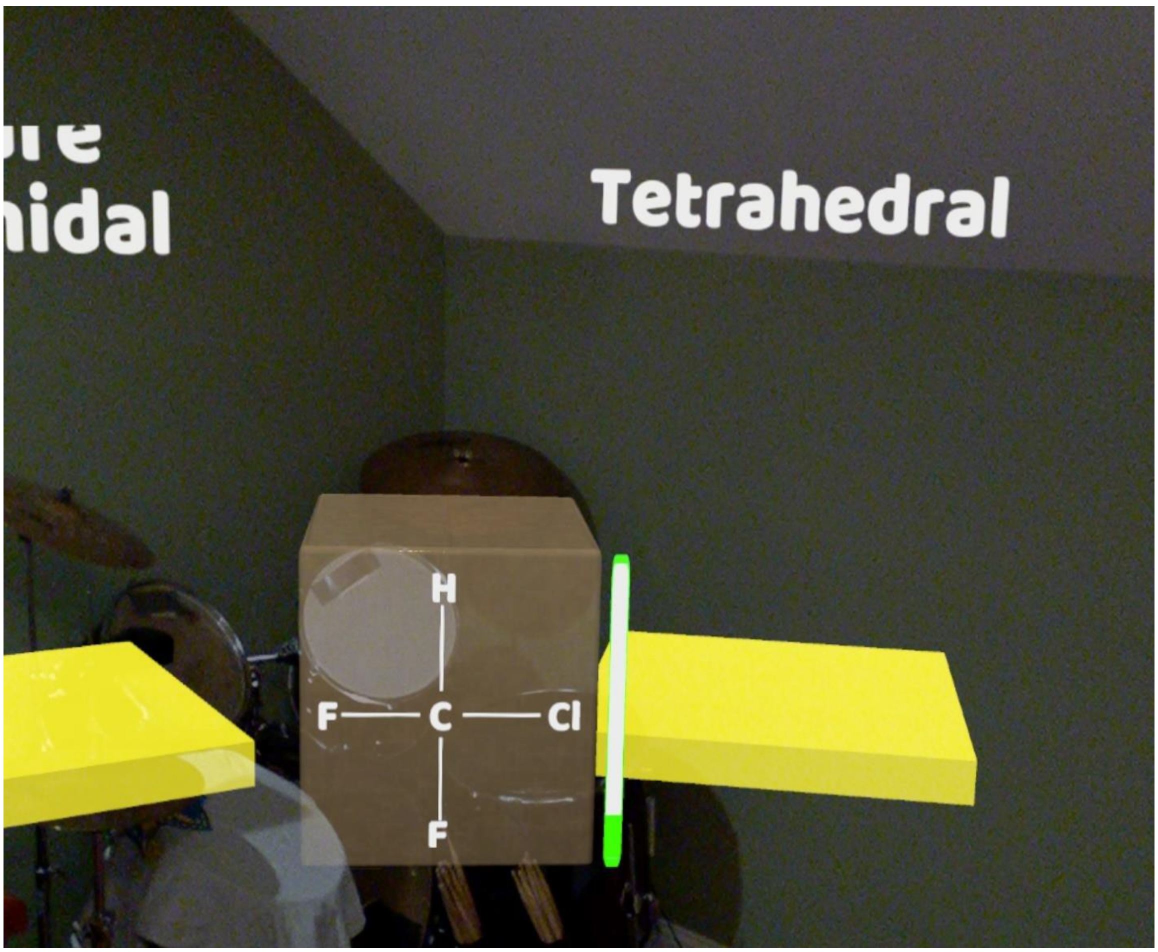

Figure 4. A screenshot from within the quiz scene of "MoleculAR Geometry." The user is presented with a box labelled with a 2D molecular structure. The user must place the box under its corresponding label. A progress bar to the right of the box indicates how many quiz questions remain.

Approach and Methods

"MoleculAR Geometry" was made in Unity, a game development engine, with coding done in C# using Microsoft Visual Studio. The molecules were designed in PyMol, a chemical visualization software, and then customized in Blender. The app was developed for the Magic Leap, an AR headset compatible with a handheld controller.

Because development for AR technologies is so new, there has yet to be established a common design for user interfaces. For now, each developer must publish her own idea on user interaction until user experience research determines a norm. Thus, this application features a fully custom menu and input system that allows for interaction between the user, controller, and virtual content. An underlying game logic script determines in-game events that follow the user's command.

Educational Decisions

The education-centered goal of this project focused on creating an application that would enhance student learning in chemistry courses such as general chemistry and organic chemistry. The application therefore requires a fusion of priorities between the software development and chemical education fields. One factor shaped by these two disciplines is the choice of device.

While VR is a more common development platform, it completely removes the students from interaction with the professor and each other. AR, on the other hand, allows the student to simultaneously experience virtual content while also discussing with peers or listening to a professor. This type of active learning and interaction between students increases learning effectiveness (Ebert-May, D. et al., 1997) and drove the decision to develop for AR rather than VR. In addition, augmented reality allows for the possibility of virtual content interacting with physical content, a technological concept known as mixed reality. For example, if a student launches a virtual ball in mixed reality, the ball would bounce off actual walls as if it were a physical object.

One of the key benefits of AR is that the user is not limited to a two-dimensional screen as one is when using a phone or computer. Content does not necessarily even need to be directly in front of the user; for a more immersive experience, the developer can place content around the physical environment, encouraging the user to walk around and explore. This concept of an interactive and three-dimensional learning environment fed into the second aim in building this application: to provide a learning strategy for molecular geometries as an alternative to the traditional table of bond angles. Rather than passively memorizing molecular facts, the students can actively inspect the molecular models, see the bond angles, and draw inferences as to how a molecule forms its specific shape. In essence, “MoleculAR Geometry” took information from a 2D table and turned it into an interactive 3D environment.

Student and Professor Feedback

As part of initial user testing, “MoleculAR Geometry” was presented to a small group of professors and students at MTSU. The participants tried the application as if they were completing an official lab assignment then gave feedback as guided by the form in Appendix A.

The surveys showed overwhelmingly positive comments on the application and its usefulness in chemistry laboratories and classrooms. Several participants noted that they preferred the 3D models in AR over traditional teaching methods with 2D models. Every student indicated an overall improvement in his or her understanding of molecular geometry, and many professors commented on the AR tool's potential for helping both visual and tactile learners. The demonstration of "MoleculAR Geometry" gained significant excitement from both invited attendees and passersby.

No participants noted any major errors or issues within the app; however, some did provide constructive criticism for the improvement of the app's user experience. Because of the limited field of view with any AR headset, a few users did not notice the content to the sides or behind them. A user interface that indicates to the user when to turn his or her head would help alleviate this problem and encourage more users to look around while using the application. One professor recommended the inclusion of space-filling models as well as the ball-and-stick models so that students could see the correlation between different types of 3D chemical representations. Several professors asked for the ability to rotate the molecule in more than one axis (currently, the app only allows for molecule rotation about the y-axis).

The comments and suggestions received from the demonstration of "MoleculAR Geometry" indicate the app would successfully aid student learning and promote student engagement in chemistry classrooms and labs. This initial user testing is vital to prepare "MoleculAR Geometry" for publication as a finished product and concludes the project's initial development stage.

Future Applications and Considerations

"MoleculAR Geometry" is a pioneer among Magic Leap apps, especially for the chemistry field. The creation of this app has opened a door into Magic Leap use for chemical education and sets a foundation on which professors might develop further apps to teach a variety of content. The application itself has immediate benefit to MTSU professors and students because of its availability in the James E. Walker Library Makerspace on each Magic Leap device eligible for check out. Future educational software developers at MTSU can also use the app's general format, functionality, and script files to incorporate AR into more classes and lessons.

Although AR-based learning increases participation and comprehension among students with neurodevelopmental disabilities such as ADHD and autism, the technology is not as accessible to other students with disabilities, such as those who are visually handicapped.

Reaching blind students is a common problem within chemistry courses, as much of the content relies on abstract drawings, visual representations, and navigation around a lab built for the sighted (Supalo, C. A., et al., 2012). Recent AR advances have led to the use of AR headsets as assistive technology for blind people by reading signs and recognizing objects (Huang, J. et al., 2019). Other chemistry labs have made use of assistive technology in the lab by providing screen readers for Vernier lab probes as well as refreshable Braille display devices (Supalo 2012). One possible accommodation for blind students when using AR in classrooms is to incorporate assistive technologies with verbal description functionality or object recognition in conjunction with physical molecular models.

While the Magic Leap was the headset chosen to carry out this project, there are a myriad of other options when deciding which AR technology to use. One device that has heavily marketed itself toward education is the zSpace, a stereoscopic 3D computer. This device comes with a stylus and glasses and encourages users to “break the screen barrier” by pulling content from the screen into the real world. The zSpace is ideal for teaching dissection or anatomy without needing any biological samples. The zSpace also doubles as a fully functioning Windows 10 computer, making it fairly easy for schools to transition from a traditional computer lab to a zSpace computer lab. Another device is the Microsoft HoloLens, a direct competitor to Magic Leap in the wearable technology industry. The primary difference between the HoloLens and the Magic Leap is that the HoloLens does not have a controller; rather, all input comes from the device’s hand tracking. The absence of a controller leaves the user’s hands free, allowing users to complete tasks such as writing or manipulating scientific instruments. However, the lack of a controller would also take away interaction with physical buttons, which users might find easier or more familiar. While each device has its differences, they all provide valuable resources for use within the classroom.

Conclusion

Educational AR technology is still in its infancy, but AR developers and educators are making strides that will make AR-enhanced education possible. “MoleculAR Geometry” is the first educational AR application for Middle Tennessee State University science classrooms. This app uses the Magic Leap headset to teach molecular geometry concepts to freshman and sophomore chemistry students while encouraging interaction and spatial reasoning. The app is free for use on MTSU Magic Leap devices, located in the James E. Walker Library.

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Appendix A: Student and Professor Feedback Surveys

On the following pages are attached the student and professor feedback questionnaires given to participants in the “MoleculAR Geometry” demonstration held at Middle Tennessee State University.

“MoleculAR Geometry” Student Feedback Survey

1. Please state your major and/or minor:

2. Before completing the demonstration, please rate your knowledge of molecular geometry from 1 (no knowledge whatsoever) to 10 (high level of knowledge).

3. After completing the demonstration, please rate your knowledge of molecular geometry from 1 (no knowledge whatsoever) to 10 (high level of knowledge).

4. What were your initial thoughts on the demonstration?

5. Do you feel that this simulation enhanced your knowledge and/or confidence of molecular geometry? Why or why not?

6. Do you think this would be a useful tool in labs or classrooms? Why or why not?

“MoleculAR Geometry” Professor Feedback Survey

1. What courses do you teach currently or have taught in the past?

2. Do you feel this simulation enhances student learning on molecular geometry and would be a useful tool in labs or classrooms? Why or why not?

3. Please list suggestions for further improvement:

4. Additional comments: