Proceedings of the Interdisciplinary STEM Teaching and Learning Conference

Volume 2 Article 3

2018

Augmented Reality Chemistry: Transforming 2-D Molecular Representations into Interactive 3-D Structures

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Keywords

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Spatial reasoning is defined as the ability to generate, retain, and manipulate abstract visual images. In chemistry, spatial reasoning skills are typically taught using 2-D paper-based models, 3-D handheld models, and computerized models. These models are designed to aid student learning by integrating information from the macroscopic, microscopic, and symbolic domains of chemistry. Research has shown that increased spatial reasoning abilities translate directly to improved content knowledge. The recent explosion in the popularity of smartphones and the development of augmented reality apps for them provide, a yet to be explored, way of teaching spatial reasoning skills to chemistry students. Augmented reality apps can use the camera on a smartphone to turn 2-D paper- based molecular models into 3-D models the user can manipulate. This paper will discuss the development, implementation, and assessment of an augmented reality app that transforms 2-D molecular representations into interactive 3-D structures.

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Recommended Citation
Behmke, Derek; Kerven, David; Lutz, Robert; Paredes, Julia; Pennington, Richard; Brannock, Evelyn; Deiters, Michael; Rose, John; and Stevens, Kevin (2018) "Augmented Reality Chemistry: Transforming 2-D Molecular Representations into Interactive 3-D Structures," *Proceedings of the Interdisciplinary STEM Teaching and Learning Conference:* Vol. 2 , Article 3.

Introduction

STEM students continue to consider chemistry one of the most difficult subjects they must complete. Johnstone states that students find chemistry difficult to grasp because they must integrate information from the macroscopic, microscopic, and symbolic domains of the discipline (Johnstone, 1991, 2000). For students to be successful, instructors must teach them to develop mental models of the microscopic interactions between atoms and molecules that explain their macroscopic observations. Chemistry instructors typically use 2-D drawings, 3-D handheld models, and computer models to ease the cognitive load associated with developing mental models (Barak, 2013; Suits & Sanger, 2013). The ability to seamlessly transition between physical models and mental models is important to student success. This ability is most commonly referred to as spatial ability or reasoning (Coleman & Gotch, 1998; Harle & Towns, 2011; Suits & Sanger, 2013).

Chemical education literature contains numerous studies that demonstrate the importance of providing students with some type of molecular model when they are carrying out tasks that require the use of spatial reasoning skills (Barak, 2013; Booth et al., 2005; Suits & Sanger, 2013; Williamson et al., 2012). Springer demonstrated that organic chemistry students who watched an instructor properly manipulate computer models outperformed their peers who did not witness the manipulation (Springer, 2014). Abraham et al. randomly assigned students to one of three treatment conditions (2-D drawings, handheld models, and computer models) to see if there was a difference in their performance on stereochemistry assessments when compared to a reference group that did not use any models (Abraham, Varghese, & Tang, 2010). Students using computer models scored 15% higher than the other treatment groups, and 37% higher than the reference group on subsequent stereochemistry assessments (Abraham et al., 2010). Kuo et al. administered a stereochemistry exam broken into subtests (Kuo, Jones, Pulos, Hyslop, & Nan, 2004). During each subtest, students used a different model type (2-D drawings, dash wedge drawings, handheld models, and computer models) (Kuo et al., 2004). Scores were significantly higher on subtests where students used handheld and computer models (Kuo et al., 2004).

Despite the overwhelming evidence in favor of using models to learn chemistry concepts, it is still difficult to convince students to use molecular models to learn concepts unless the models are provided by the instructor. The explosion in popularity and availability of smartphones and augmented reality technology may provide a means to bridge this gap.

Augmented reality is a technology that virtually overlays information or interactive elements on top of a mediated view of the user's physical environment. A computing device with a camera and a screen, typically a smartphone or tablet, provides the mediation. The user points the device's camera at an object that acts as a trigger in the physical environment, and virtual elements are added to, or over, the object on the device's display. The virtual elements are, in their simplest form, an active element such as a video. In more complicated forms, the trigger can be overlaid with user interface elements and/or 3-D constructs. One example of such a construct is a 3-D molecular model a user can manipulate. (Delello, McWhorter, & Camp, 2015; Dunleavy & Dede, 2014; Ke & Hsu, 2015)

DOI: 10.20429/stem.2018.020103

A number of augmented reality platforms have been developed and used in the educational arena; however, this field is not particularly mature (Dunleavy & Dede, 2014; Figueiredo, Gomes, Gomes, & Lopes, 2014). A number of investigators have used various augmented reality platforms to research artifact creation in college classes, including the areas of teacher education, business, and marketing (Delello et al., 2015; Ke & Hsu, 2015). Though augmented reality may already have a role in some chemistry classrooms, no literature could be found documenting its use. Can an augmented reality based molecule viewing app be developed that can provide students with a mobile, technology based solution to enhance their understanding of chemistry?

App Development

For an initial proof of concept of the augmented reality molecule viewing app, the platform Aurasma was selected. Aurasma is one of many augmented reality platforms that has been previously used in educational settings. Non- commercial use of this platform is free, and it provides apps for both Android and iOS mobile devices. It has operated for a number of years and provides a reasonable degree of stability. It also provides a straightforward web-based authoring environment for creating augmented reality artifacts, referred to as auras. (Figueiredo et al., 2014) Given these characteristics, the majority of the development work focused on creating a process to generate and view 3-D molecular representations using this platform.

The process of generating a 3-D molecular aura that a user could manipulate involved a series of steps; first, generating a 2-D drawing of the molecule that was to be displayed. This drawing ultimately served as the trigger that later initiated the augmentation when the mobile device's camera driven by the app was pointed at it. A .mol file of the molecular structure was then generated using a molecular drawing program such as ChemDraw. The .mol file was then converted to a protein database (pdb) file, which was subsequently converted to a 3-D molecular structure using the free, open source 3-D creation suite Blender. The 3-D structure file was then transferred to Aurasma Studio and linked as an overlay to the 2-D drawing to create the aura. At this point additional overlays, such as buttons to allow molecular rotation, were added to the aura to enhance the user experience. Finally, the aura had to be shared so that end users could access the experience. In order to access the augmented reality based auras, users would download the Aurasma app and follow the channel where the auras were shared. Once the user followed the appropriate channel, they simply opened the app and pointed the camera on their mobile device at the appropriate 2-D drawing trigger.

Implementation and Assessment

Stereochemistry has long been recognized as one of the more difficult topics in organic chemistry courses, because distinguishing between pairs of 2-D molecular drawings without an algorithmic approach requires a great deal of spatial ability. The first augmented reality based activity that was developed, and Institutional Review Board (IRB) approved, sought to enhance student learning in this area. The activity, which was designed to take no more than ten minutes to complete, is shown in Figure 1.

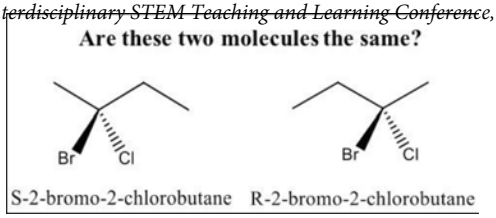

Figure 1: The first stereochemistry augmented reality based activity developed. *(Note: Molecule names were omitted in student version)*

The activity was implemented in several sections of organic chemistry I during four different terms (spring 2016, summer 2016, fall 2016, and spring 2017). During each term, there were an equal number of randomly assigned experimental and control sections, which resulted in total of 238 student participants (control N = 116, experimental N = 122). Instructors in both the experimental and control sections were asked to incorporate the activity near the conclusion of their normal instruction on stereochemistry, and students were permitted to discuss their answers with each other. In control sections, the activity was completed as a paper and pencil exercise that concluded with the instructor discussing the correct answer. Students in control sections were permitted to use model kits if they had them during the activity, but no student elected to build models. In the experimental sections students first downloaded, installed, and setup the Aurasma app, and then they were told that the image in Figure 1 above, with the molecule names removed, was a trigger to begin an augmented reality experience. The experience allowed students to view side-by-side 3-D representations of the drawings in Figure 1 which they could rotate by pushing a button on their screen. Additionally, they could push a button and see a video explaining the correct answer. At the conclusion of the activity both experimental and control sections completed the same assessment.

The assessment asked students to indicate whether pairs of molecules were the same (identical) or different (enantiomers or diastereomers). Experimental section students were not permitted to use the app on the assessment. All students were permitted to use their own model kits on the assessment, but none did. During the assessment students were also asked which type of model (handheld, computer/app, both, or neither) would have assisted them in better learning the stereochemistry material, and they were asked to briefly explain their choice.

Results and Discussion

Students in the experimental sections had an average score of 68.0% on the assessment, compared to 63.3% for students in the control sections. A t-test showed that these results were not significantly different ($p = 0.12$). These results are not surprising considering students only participated in one ten-minute activity prior to completing the assessment. These findings, however, suggest that the inclusion of the augmented reality activity did not negatively impact student learning. These results, combined with the enthusiastic response of the students as they interacted with the Aurasma app, indicate that augmented reality based molecular models have a future in the chemistry classroom.

The positive student performance results are further validated when their opinions

DOI: 10.20429/stem.2018.020103

of model types are examined. Figure 2 summarizes student opinions of useful model types to learn stereochemistry material broken down by experimental and control sections.

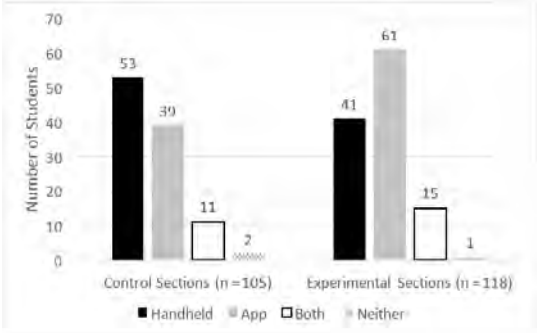

Figure 2: Student opinions of useful model types to learn stereochemistry material broken down by experimental and control sections.

Students in the control section preferred handheld models (N = 53) over computer or app based models (N = 39). Student explanations indicated that they did not believe computer models were tactile enough, and that they did not believe computer based models could accurately depict 3-D structure. Students in the experimental sections preferred computer based models (N = 61) over handheld models (N = 41). Students preferred the computer based models because they accurately portrayed 3-D structure, it was easier and faster to access them compared to constructing handheld models, and they did not have to carry around a physical model kit. Students in the experimental section who still preferred handheld models cited the lack of tactile interaction as the app's number one weakness. Notably, all students in each section are required to have physical model kits, but no student in either section used these, even though they are highly encouraged to use them for the same reasons noted by student feedback.

When the performance data is combined with student opinions regarding the app, it becomes clear that augmented reality based molecular models have a role in the chemistry classroom. In order to provide a more definitive answer regarding their impact on student performance, a more detailed and rigorous set of augmented reality based activities will need to be developed, implemented, and assessed. Additionally, modifications will need to be made to the app experience to enhance tactile interactions the user has with the models. Work by McCollum et al. validates the need for more tactile interactions by demonstrating the that users equipped with an iPad's touch screen to interact with models showed superior representational competence compared to their peers who used 2-D paper drawings (McCollum, Regier, Leong, Simpson, & Sterner, 2014).

Conclusions

An augmented reality based molecule viewing app that can provide students with a mobile, technology based solution to enhance their understanding of chemistry was developed. The process for developing 3-D, augmented reality based molecular representations from 2-D, paper-based drawings is time and developer intensive. Nevertheless, students using augmented reality models perform at least as well as those using no models. Students who have used augmented reality models find them more

convenient and faster than traditional, handheld models, and more students would prefer augmented reality models if they were more tactile, meaning the user had greater control over molecular manipulations.

Current and Future Work

As work progressed, it became increasingly apparent that the selection of Aurasma as the platform for the app came with some serious limitations. The freely available, non-commercial package necessitated a cumbersome and time intensive process for generating the augmented reality based molecules. Given the large number of molecules end users would want to use, this is a significant hurdle. Additionally, the platform provided no seamless way to increase the tactile interactions with the models, which both the initial pilot testing of this app and the work by McCollum et al.(McCollum et al., 2014) suggests would be desirable and beneficial to the user experience. In order to alleviate these deficiencies, it became apparent that a standalone augmented reality app developed specifically for the intended use in a chemistry classroom was needed.

The development of such an augmented reality molecule viewing app is well underway. The Android and iOS app is currently in beta testing. The app uses 2-D drawings of molecules as triggers, much like the Aurasma app. The 3-D molecular structure is retrieved from the PubChem Database and is dynamically converted to a 3-D model that is presented to the user to generate an augmented reality experience. This automated process only requires the development of a trigger for each molecule. Users can rotate molecules using their fingers, and they can use pinch gestures to zoom in and out. Both of these features increase the tactile interactions users have with the models. The app also provides a color key, which clearly identifies the type of atom(s) in each substance. Assuming successful pilot testing, the app should become more widely available in the near future.

One of the more recent technologies to burst onto the scene are mixed reality headsets, such as Microsoft's HoloLens. These headsets have a wider viewing angle. This will allow the user to view larger numbers of more complex molecules in greater detail. We have designed a prototype molecule viewing app for the HoloLens. This app does not use a trigger but rather allows the user to directly select the molecule(s) he/she wants to view from a pre-populated list. The 3-D molecular structure is retrieved from the PubChem Database and automatically converted to a 3-D model. Users can zoom in and out and rotate molecules with both hand gestures and speech. The HoloLens app will enter beta testing soon.

Acknowledgements

This project was supported by funds from a USG-STEM Initiative II Mini- Grant and a Georgia Gwinnett College SEED Grant. Special thanks to the faculty of the chemistry and information technology disciplines at Georgia Gwinnett College who volunteered their expertise and class time to help with the project.

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DOI: 10.20429/stem.2018.020103

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