AR-some Chemistry Models: Interactable 3D Molecules through Augmented Reality

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ABSTRACT

Augmented Reality (AR) presents many opportunities to design systems that can aid students in learning complex chemistry concepts. Chemistry is a 3D concept that student soften have trouble visualizing using 2D media. AR-some Chemistry Models is an AR application to visualize complex chemical molecules. Our app can generate 3D interactive molecules from chemical names, hand-drawn and printed line-angle structures of complex molecules. Allowing for handwritten input gives a student instant feedback on their self-generated understanding of a molecule and can improve knowledge retention. Students have the opportunity to visualize molecules from lecture notes, or even homework problems. Our application allows the student to interact with this molecule using simple touch screen commands to zoom in, zoom out, rotate and move the molecule in AR to understand the spatial relationship among the components. Our application also highlights and displays relevant textual information about a molecule's functional groups when they are tapped to further improve student learning. We present an affordable and accessible study tool to help students with their learning of chemistry molecules.

CCS CONCEPTS

• **Human-centered computing → Mixed / augmented reality**.

KEYWORDS

HCI, Augmented Reality, Chemistry, Molecules

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1 INTRODUCTION

The structure and shape of complex organic molecules is a vital concept that students must understand when studying chemistry. Students often have trouble visualizing 3D molecules when presented as 2D drawn molecules. We envision augmented reality as an affordable and accessible way to enrich molecular visualization and understand their interactions.

The typical method to visualize these molecules in 3D space is for a student to use a physical "ball and stick" model kit. These kits include colored "atoms" that can be "bonded" using plastic pegs and are (usually) able to accurately demonstrate bond angles within the molecule. Building these "ball and stick" models does not provide immediate feedback for the students to visualize their drawn 2D molecule. Students also do not receive feedback on whether or not their constructed molecule is even correct. Additionally, these kits have physical constraints limiting the complexity of the molecules that can be visualized as a result of limited balls and sticks.

A potential solution to this would be to allow the student to view molecules in 3D using their phone or computer, but the utility of simply looking at different 3D organic molecules is also limited. While it does remove physical limitations, this method also removes most benefits that a physical model would have: kinematic response, experiential learning and partial feedback.

AR-some Chemistry Models strives to bridge this gap in chemistry education by turning 2D chemistry molecules into interactable 3D molecules through augmented reality, while providing opportunities for user interaction, experiential learning, and educational feedback. AR-some Chemistry Models aims to supplement student's study of chemistry by visualizing hand drawn molecules as well as their printed counter-part and the chemical name. Students can compare their drawn version for real-time feedback and can create engaging/useful note cards or study guides. Students can also visualize models by pointing their mobile device at lecture slides or the textbook or even on their homework problems. Study material content appears as an overlay when parts of the molecule are selected. AR-some Chemistry Models enable quicker access to a 3D model, and also aids the student in making the connection between the 2D representation and the 3D model more effectively. The interactivity and user control of the molecules presented in AR should further aid in student learning and knowledge retention.

2 RELATED WORK

2.1 Visualizing Complex Structures

Several researchers have created apps to generate 3D molecules based off of 2D image targets. [5] created an AR application using Unity and Vuforia designed to help students understand complex molecular chains and crystalline structures. To show more simple molecules, [13] developed an AR app using Google Sketch Up, Corel Draw X5, and Unity 3D to display the BrF_5 molecule and tested student comprehension with a worksheet. Other similar projects such as [11] and [2] also use a concept of AR target print outs to aid in learning by showing students a relationship between a 2D image and a 3D molecule.

These systems were designed to generate a 3D representation of a molecule using image targets consisting of generated QR codes with no correlation to the models being generated, or preset image targets which leaves out the learning opportunity of students hand generating their molecules. We aim to increase interactivity and strengthen the understanding between the 2D line-angle molecule and the 3D visualization shown in our AR app. Our application shows the 3D molecule through recognition of multiple image targets including: 1) word text, 2) pre-printed line-angle targets, and 3) drawn line-angle targets. In addition our models differ from others by utilizing CPK color coding and precisely accurate bond angles to deliver a comprehensive and accurate representation of the material.

2.2 Interacting With Molecules

Embodied learning is gaining traction in STEM education [8]. This means that students' actions are part of learning and designed into the lesson. Significant knowledge increases have been seen in fields as varied as math [10], physics [7] and astronomy [15]. As the team designed this chemistry content the goal was to make it based on the learners' hand-drawn line-angle output, it was also important that learners have control over the orientation and level of detail of the molecule.

Works from Aw et al. [3] developed an application that allows users to manipulate 3D chemical compounds and simulate a nucleophilic addition reaction on a molecule in AR. To interact with the model, students would aim with their fingers to generate the valid reaction. This work specifically focuses on a combination of two specific molecules and is limited in content. Maier et al. [12] created two hand-held image target depicting simple geometric black and white patterns that act as a landing pad for 2 molecules. This system uses the two hand-held image target requires the physical movement of the image target to manipulate the resulting 3D molecule.

Our application displays informational overlays about the molecules and highlights parts of the molecules when tapped. Through our highlighting feature, AR-some Chemistry Models provide information about the molecules in a way in which the works mentioned earlier do not. While the molecule is highlighted and the information is displayed, the user can still manipulate and move the molecule.

3 DESIGN AND IMPLEMENTATION

Our goal is to create an engaging and effective chemistry study tool utilizing augmented reality to transform 2D line-angle molecule structures into 3D structures. AR-some Chemistry Models can recognize, the chemical name, hand-drawn and pre-printed line-angle molecule structures. Students are able to hand-draw their line-angle molecules on hexagonal graph paper and visualize the 3D molecules immediately after. Not only can students visualize these molecular structures, but they can also interact with them as well, i.e. rotating, moving, pinch zoom-in or pinch zoom-out. Tapping on the respective subgroups of the molecule highlights and showcases relevant chemistry information to aid in studying. To our knowledge, we offer the only AR chemistry overlays that allows users to seamlessly alternate between whole and subgroup displays.

3.1 The Molecules

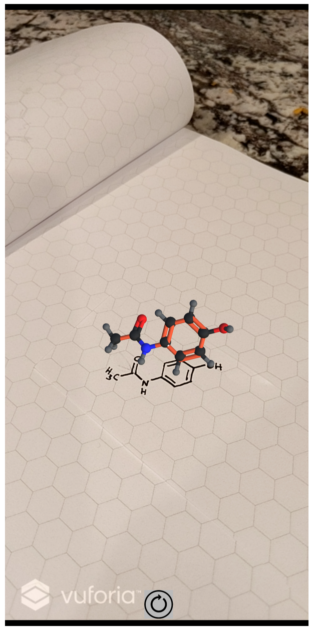
To create the molecule database, the team used jmol, blender and Unity 2019. Using jmol, almost any molecule with an IUPAC name can be found in a 3D and 2D format. After searching for a desired molecule, the molecule is exported as a jmol object to Blender. Here, the molecule is edited to retain correct shape, show proper atomic angles, have correct CPK coloring scheme, and is given aesthetic touch ups such as reflectivity and smoothness. Once the 3D object has been properly transformed, it is then exported as an .obj file into Unity where it can be used in the AR app. After being repeated with a number of different organic molecules, this library of models is planned to be made open source in the .obj format. In addition, subcomponents of larger molecules can be taken apart and reassembled into new molecules quickly within Unity.

3.2 Augmented Reality Application

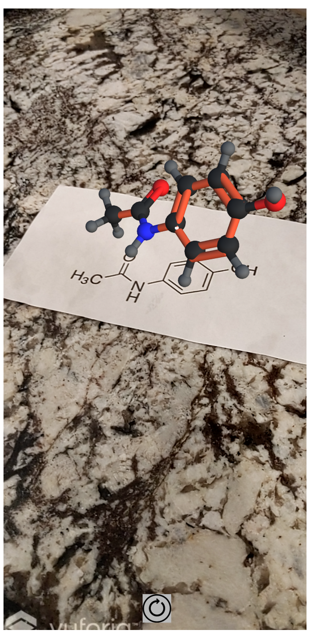
Our application offers visualization of a 3D molecule though three different image target methods: using word targets, pre-printed line-angle molecules, and hand-drawn line-angle molecules. The scenarios are shown in Figure 1. For word targets, a printed note-card with the name of a chemical compound using size 36 Elephant font will be used. For printed line-angle molecules, a line-angle molecule is printed onto a sheet of paper. For drawn line-angle molecules, a line-angle molecule is drawn onto hexagonal chemistry graphing paper. If the molecule is drawn correctly, then a 3D molecule will appear. If drawn incorrectly, nothing will show. The hexagonal paper acts as a guide to ensure straight lines and proper molecular angles similar to the image targets associated with the molecules (but it is not a necessary condition). After scanning the image target, the corresponding 3D model for the molecule will appear on the device screen. In an embodied manner, the user can now in which users can manipulate, rotate, and select various parts of the virtual model.

The AR-some Chemistry Models application runs on an Android device running Android 11. The current AR software being used for this app is Vuforia AR created by PTC. The software is configured such that when a either the word target, pre-printed molecule or drawn molecule is detected, the corresponding .obj 3D object is displayed from a molecule library.

(a) Visualization from word target



(b) Visualization from hand drawn molecule



(c) Visualization from printed molecule

Figure 1: AR-some Chemistry Models use cases

3.3 Interactions

The molecules in the app can be manipulated, i.e. moved, rotated, zoomed in, and zoomed out. These manipulations allow a user to not only visualize the molecule in 3D but to choose different angles and zoom into certain substructures of the molecules if the user wants to. Users who have control over their angles of view in 3D space learn more than users who were assigned to passively observe prechosen views [6]. The position and orientation of the molecule is tracked, so if a student wants to view another molecule and return to a previous one, their manipulation is saved. The molecule can even be taken away from the target and moved to a different position in the room if desired.

When the user taps specific parts of the molecule, the corresponding functional group highlights and an information overlay appears. This is shown in Figure 2. The user can still manipulate the molecule while the portion is highlighted.

If students make their molecule too small or too large to properly analyze, remove the highlighting, there is a reset button present at the bottom of the screen to reset the molecule to the original state. Multiple different molecules can be generated and compared at once, aiding students in studying subjects like stereochemistry and chirality.

4 FUTURE WORK

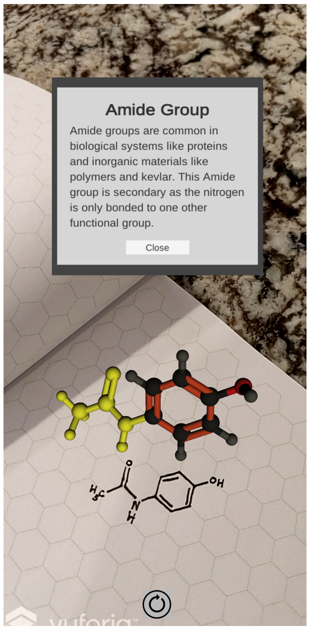
The plan is to continue development to improve the highlighting feature in the application. Users can select different individual components of the 3D molecule to have that portion highlighted. Once the component is selected, the same portions would be highlighted in the 2D molecule to showcase the relationship between the 3D and 2D model. There are also plans to turn this application into an interactive quizzing tool with embedded questiosn like "Where would the next carbon attach in order to make X molecule?" Students would then tap the appropriate bond area and the immediate feedback would be given.

We also plan on implementing virtual translucent overlays of the line-angle molecules. Students can actively practice how to draw the line-angle molecules more accurately and effectively.

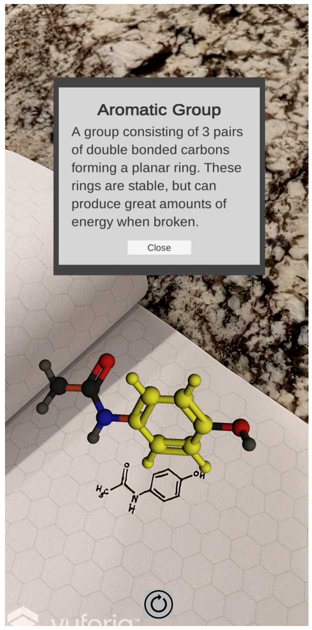
A longer-term goal is to have AR-some Chemistry Models used in a full course of chemistry curriculum. We plan on expanding the number of molecules recognized to fit the educational modules and curriculum. Next year, a mixed methods study will analyze educational outcomes of students studying chemistry using our system compared to more traditional methods. We plan on making our 3D models and image targets open source for broader educational dissemination.

5 CONCLUSION

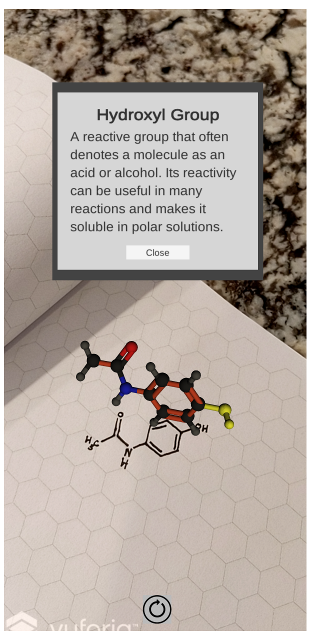
In conclusion we present AR-some Chemistry Models, an augmented reality application to visualize chemistry molecules. AR-some Chemistry Models seek to empower and embody students who are studying chemistry by providing 3D visualization and interaction capabilities for chemical names, pre-printed and drawn line-angle molecules. This high fidelity application should make it easier for students to connect the relationships between 2D and 3D versions of the molecules when studying chemical molecules. We plan to further develop and study the effects of this application to further understand how it might educational outcomes in chemistry.



(a) Selected Amide Group



(b) Selected Aromatic Group



(c) Selected Hydroxyl Group

Figure 2: AR-some Chemistry Models information overlay

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