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Technology Report

MoleculAR: An Augmented Reality Application for Understanding 3D Geometry

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ABSTRACT: MoleculAR is a free, multiplatform augmented reality (AR) application that allows students to visualize and manipulate molecular structures in 3D, providing a more immersive and interactive learning experience. Using QR codes to generate 3D models of molecules, geometries, and orbitals, students can explore structures in real-time using their smartphones or tablets. Based on student survey responses, the app is effective at engaging students in both first- and second-year chemistry courses. Our goals for MoleculAR include providing a universally accessible tool for students to learn about molecular geometry and allowing for instructor adaptation and customization to make it as relevant as possible for individual courses. The skills students develop with the help of the app are highly transferable to other topics or areas, making it a valuable resource for educators in other fields. We welcome other educators to adopt the app to facilitate their teaching and improve the learning outcomes for their students.

KEYWORDS: *General Chemistry, Introductory Organic Chemistry, Molecular Structure, Augmented Reality, Molecular Modeling, Stereochemistry, Teaching and Learning Methods, Computer-Based Learning*

INTRODUCTION

Molecular Geometry and Its Significance

Learning chemistry requires the ability to integrate information from the microscopic domain of molecules, atoms, and orbitals through the macroscopic domain of experiments and demonstrations while navigating the symbolic domains of chemical and mathematical representations. These three domains are part of what is known as Johnstone's triangle.[1] While experts have the ability to swiftly shift between the three domains, first- and second-year chemistry students often have difficulty navigating the triangle.[2]

The three-dimensional (3D) depiction of molecules and their stereochemistry is one of the most difficult chemical concepts for students to learn and for educators to teach.[3] The ability to visualize molecules in 3D facilitates student learning by bridging the symbolic structures we draw on paper with the microscopic atomic properties from which, ultimately, macroscopic experiments can be designed and understood. In the past, teaching 3D visualizations in chemistry has benefited from the use of physical models such as ball and stick molecular kits.[4] These tools have been shown to help students better understand molecular transformations and make the connection between 3D chemical structures and reactivity,[5] with visual literacy and visualization serving as key learning mechanisms.[6,7]

Advancements in AR Educational Technology

New technologies are redefining learning experiences in the 21st century, with the growing implementation of computer-based programs for 3D molecular visualization, allowing students to interact with complex structures and processes in a more immersive and intuitive way. Augmented reality (AR) technology has emerged as one example of a visualization method that is capable of creating real 3D models. Many people are already familiar with it in nonacademic contexts, such as gaming, where they can discover and battle virtual creatures in Pokémon Go, selecting tattoos, where they can superimpose them on their body using Inkhunter, ensuring that furniture fits and matches in their home, as with Ikea Home, and all manner of measuring tools. More recently, this technology has been increasingly utilized in education to enhance student learning experiences.

AR has had a presence in the chemistry education literature for a little over 10 years,[8] though many of the tools are

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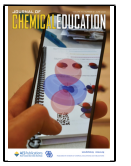

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proprietary and/or designed for applications other than understanding 3D geometry. Examples include colorimetric titrations,[9] analytical instrument design,[10] macromolecular function,[11] elemental properties,[12] escape games,[13] DNA precipitation,[14] and many more. When AR is used to visualize and interact with molecular structures, it can provide students with a better understanding of the 3D geometry and molecular properties. For example, AR has been used to create interactive simulations of chemical reactions, allowing students to observe and manipulate the reaction in real-time.[3]

However, many existing AR applications in chemistry are limited in scope, functionality, and accessibility. Recent work providing guidance for making an AR app has been published in an attempt to make AR implementation more accessible, regardless of programming skills, using free software.[15] However, this software is specific to Android devices, which was problematic for our students since approximately 85% of them own Apple devices. Other approaches are also often limited to one platform only.[16−18] Static 3D models in some apps also pose challenges associated with the limitations of student understanding of depth cues in molecular structure.[19]

In the realm of AR education technology, it is important to consider the various applications available and their specific functionalities. NuPOV stands out as an excellent free-to-use mobile AR app allowing students to explore reaction mechanisms, although its focus is limited to simple nucleophilic addition reactions.[20] On the other hand, molAR offers the capability to visualize molecules in AR directly from hand-drawn chemical structures or protein data bank IDs.[16] However, it is not QR code linked, which is a requirement for us to provide a strong link between the printed coursebook and the app. MoleculAR uses QR codes that allow educators to set the molecules that students engage with, serving as an extension of the coursebook. Additionally, MoleculARweb is another outstanding, free, open-source web-based app with interactive AR capabilities, offering a wider range of functionality.[21] However, the augmented reality in MoleculARweb is either a sandbox for exploration or a structured lesson that cannot be adapted to specific instructor needs.

Additionally, many apps have been developed but have simply vanished from the iOS and Android App Stores. There was in fact an app called MoleculAR that had similar properties to our own, but it is no longer available or supported.[22] Our MoleculAR app was developed completely independently from the defunct MoleculAR app developed by Coster, which coincidentally had the same name. The discovery of the existence of the previous MoleculAR app was made after our MoleculAR had already been developed.

Objective of the Study: Development of AR App

The specific functionalities and limitations associated with available apps are frustrating for the desired outcomes of our courses. We cannot reliably use a tool that is not universally accessible or ceases to exist midcourse, and we would dearly like to customize the tool to make it as relevant as possible for our own students while making it available for others. To address these limitations, the MoleculAR project was conceptualized as an augmented reality application specifically designed for chemistry education. The app was developed to allow students to visualize and manipulate molecular structures in 3D, providing a more immersive and interactive learning experience. The MoleculAR app builds on previous work in the field of AR education in chemistry, including the use of QR codes to link to AR representations of molecules and structures. It expands on these previous efforts by incorporating a wider range of molecules and atomic orbitals. What sets MoleculAR apart from other examples is its cross-platform compatibility, ease of use, and streamlined nature with the QR code interface, allowing the app to serve as an aid to the lesson without potentially detracting or diverting focus.

In this paper, we describe the development and implementation of the MoleculAR app as well as its reception among first- and second-year chemistry students. We also discuss the potential impact of the app on student engagement outcomes and its potential for broader applications in chemistry education. Overall, the MoleculAR app provides students with a more engaging and effective learning experience.

METHODOLOGY

App Design and Development

MoleculAR was developed using Unity 3D, and the AR foundation package was developed with ARCore and ARKit for Android and iOS development, respectively. Molecules and their geometries were first generated in Avogadro and then converted to MOL files which were then imported into Unity via a custom script for converting MOL files into matching Unity 3D prefabs. The use of Avogadro and MOL files was integral to the development of MoleculAR. Avogadro allowed for a broad variety of molecules to be generated from various sources, including existing XYZ geometry files and newly created geometry files. After optimization of the structure geometry energies at an educational level using Avogadro, the challenge was to transfer these geometries into Unity 3D. Here, MOL files were chosen due to their regular structure, well-documented lists of atoms and their coordinates, and the inclusion of atomic bonding information. This choice enabled the seamless generation of a 3D structure within Unity 3D that accurately represented the generated geometry. Atomic orbitals were created in Blender 3D using a custom Python script that simulates orbitals as generated by their wave functions.[23] A custom script written in Processing 3.0 generated the QR codes. The QR codes do not encode a link or information but instead serve as points of interaction. This choice to use QR codes as points of interaction was due to their high visual contrast, making them ideal as real-world objects for software to track.

The basic functioning of the app is as follows. Upon launching the app, the student sees an interface with two options: START and HELP (Figure 1a). By choosing START and scanning the QR code with their smartphone or tablet device, the app generates the corresponding 3D model that appears to hover within the real-world space of the viewer (Figure 1b). The user can then interact with the model using simple finger gestures to rotate, zoom, and inspect the model closely, with user instructions available under the HELP option (Figure 1c). When an animation is generated, it can be scrubbed through by the user or allowed to play naturally. The user also has the option of switching between space-filling or ball-and-stick representations of the structures and toggling the visibility of the lone pairs on the structure.

The MoleculAR app was designed with the goal of creating an intuitive and user-friendly interface for students with a focus on user-centered design principles. The use of point-of-interaction QR codes that link to 3D models provides students

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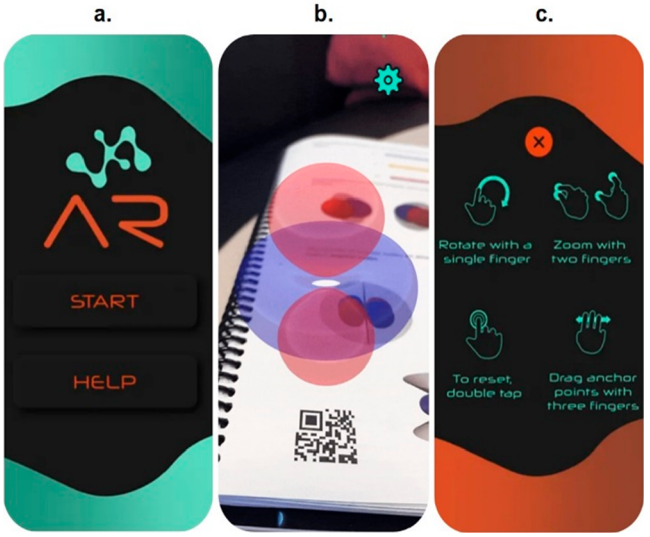

Figure 1. Smartphone screenshot of (a) MoleculAR START page, (b) example 3D d_z^2 orbital as it appears floating above lecture textbook QR code, and (c) HELP options for how to manipulate 3D models.

with a familiar access point to spatial-structural learning and engagement via their smartphones. The QR code library can be downloaded for free at https://chagunda.github.io/moleculAR/. This allows any user, whether it be a curious user looking to explore molecular geometry or other educators wishing to incorporate MoleculAR into their course, to access the library without the need for the course lecture book.

Classroom Implementation

The app design process also involved extensive small-scale testing and refinement with feedback from both students and colleagues. MoleculAR was initially tested at scale by students in the first-year introductory chemistry course (CHEM 101) at the University of Victoria. This feedback was used to inform the development of new features and improvements to the app with a focus on maintaining simplicity and ease of use. This testing was extended to second-year organic chemistry (CHEM 231) by adding more molecules and atomic orbitals, which also require comprehension in a 3D context.

Implementation was straightforward; QR codes were embedded into the students' lecture books, and when the instructor encountered a QR code, students were prompted to open the app. On the first encounter, the instructor gave the students a brief tutorial on the use of the app. We found that the students used the app with ease, being familiar with the appropriate gestures and intuiting much of the functionality even without reference to the help function. While we did not dwell too long with the app on any particular structure, we frequently encouraged the students to use it to help their comprehension of 3D objects. The response was gratifyingly positive, as evidenced by both the survey results (vide infra) and the general atmosphere in the classroom, with expressions of delight and surprise and an excited hum as the first students got it to work and showed their neighbors.

MoleculAR has additionally been developed with accessibility and customization in mind by enabling educators from other institutions to contribute molecules or 3D models. Addition requests can be made via email to the authors, with any MOL file being compatible for addition, while any 3D models can be incorporated if importable into Blender. New request additions to the app will be updated in batches every three months, allowing ample time for integration into course books or lesson plans. Figure 1b shows an example of how MoleculAR can be incorporated into a course book. Educators can easily download and insert QR codes of their requested structures into their own course textbooks and materials, allowing them to take advantage of MoleculAR in their own teaching. Additionally, a review sheet of molecules with names, images, and QR codes has been generated for easy reference and is available on the GitHub host site.

Targeted Learning Objectives

The MoleculAR app was designed with the hypothesis that it can help students learn about molecular structure and bonding using AR, with learning objectives developed from but not limited to the CHEM 101 curriculum. One of the topics is the quantum mechanical description of electrons in an atom using three-dimensional wave functions or orbitals. It is hypothesized that, using MoleculAR, students will be better equipped to predict the structures of small molecules using valence shell electron pair repulsion (VSEPR) theory. With this visualization aid, students can then explain the concept of atomic orbital

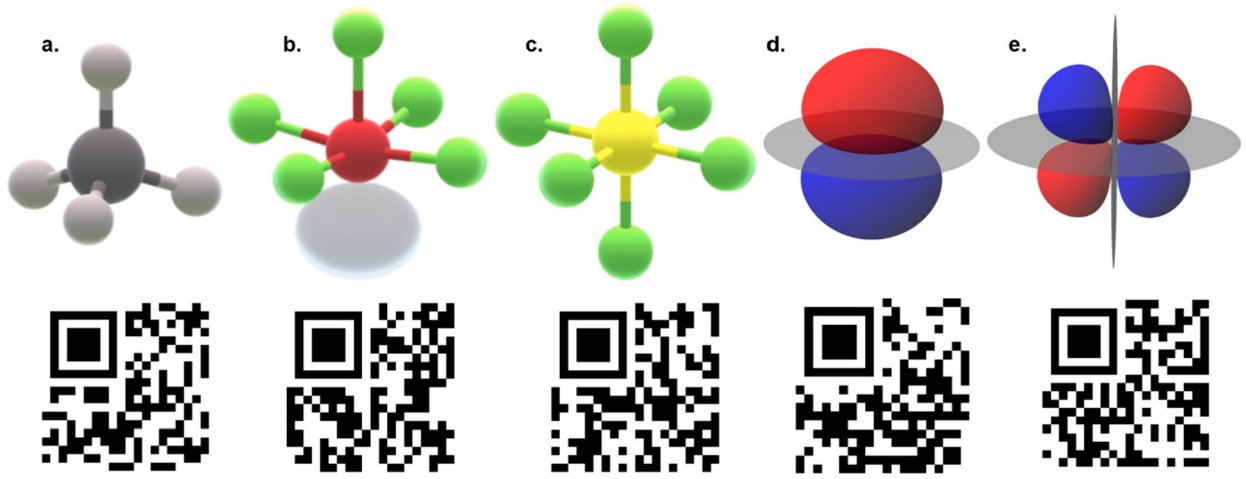

Figure 2. Examples of MoleculAR 3D structures of (a) tetrahedral, (b) square pyramidal, and (c) octahedral geometries as well as (d) p_z and (e) d_{yz} orbitals, with associated QR codes.

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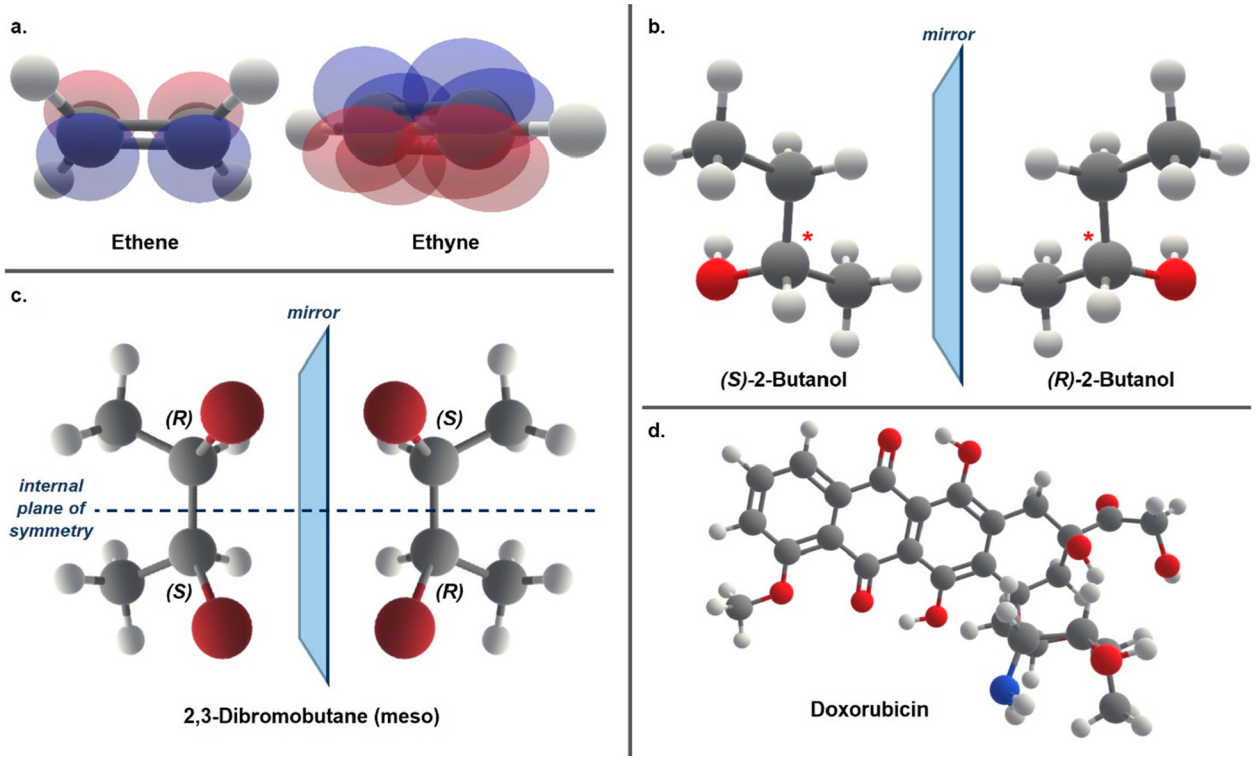

Figure 3. Examples of complex structure visualization using MoleculAR including (a) p orbital overlap in ethene and ethyne, (b) stereoisomer nonsuperimposability of 2-butanol, (c) mesosymmetry in 2,3-dibromobutane, and (d) structural complexity of doxorubicin.

hybridization and its relation to various molecular geometries. Additionally, the 3D models may enable a more visual introduction to concepts of chirality and the properties of a molecule that allow it to have enantiomers. Figure 2 shows some examples of 3D geometries and orbitals that can be explored by using MoleculAR.

It is also hypothesized that students may be able to better outline the basic approach to deriving molecular orbitals from atomic orbitals and describe the traits of bonding and antibonding molecular orbitals through the visual aids provided by MoleculAR. All of these learning objectives require an appreciation of 3D geometry, and without that understanding, students may struggle to progress in their conceptual understanding. The app is hypothesized to have the potential to enhance students' conceptual understanding and interest in chemistry.

Accessibility

The app design was informed by the principles of Universal Design for Learning (UDL), which emphasize the importance of creating learning experiences that are accessible to all students, regardless of their individual needs or abilities.[23] To this end, the MoleculAR app was designed to be compatible with a wide range of devices including both iOS and Android platforms.

Our surveys of students enabled us to examine whether there are any accessibility-related issues with the app. The aim was to offer alternatives to any students who report difficulties, such as visually impaired students and students who do not possess a smartphone, two constituencies of which we are aware of, and there may be others. To address these limitations, we are continuing to use our physical models for students,[24−27] and these will remain a free addition to our lecture materials for the foreseeable future.

RESULTS AND DISCUSSION

MoleculAR was developed in 2021 and introduced to our classrooms during the Fall semester of the same year. The app is used by approximately 900 students in CHEM 101 and 600 students in CHEM 231 per year. The use of MoleculAR in introductory organic chemistry allowed us to move from single atoms to molecules. Thus, students were able to visualize π bonds in double and triple bonds, chirality, and symmetry elements (Figure 3). Having the p orbitals visible in ethene and ethyne, students could conceptualize the perpendicular relationship between the plane of the sigma framework and that of the π bond (Figure 3a). This streamlined the process of predicting and drawing addition-reaction products. MoleculAR was also used to explain stereoisomer nonsuperimposability (Figure 3b) and the plane of symmetry in *meso*-compounds (Figure 3c). The largest molecule in our collection so far is doxorubicin (Figure 3d), which we use to introduce students to the complexity of organic structures with real-world applications.

We conducted a survey of the students' qualitative impressions of the app with the CHEM 101 and CHEM 231 classes of Fall 2022, receiving 123 responses. Participation in the feedback survey was fully voluntary, and thus, many students decided not to participate. Therefore, the responses may not fully represent the entire student population. However, of the students who did respond to the survey, the majority had positive feedback. 88% of respondents replied to the question "Did you use the MoleculAR app?" in the affirmative. Some student responses included the following: "*Overall, an excellent addition to the Chem 231 teaching team :)*", "*Very cool and fun to use!*", and "*It was surprisingly good*".

In addition to app adoption, students were also asked to evaluate the utility of the app. They were tasked with rating

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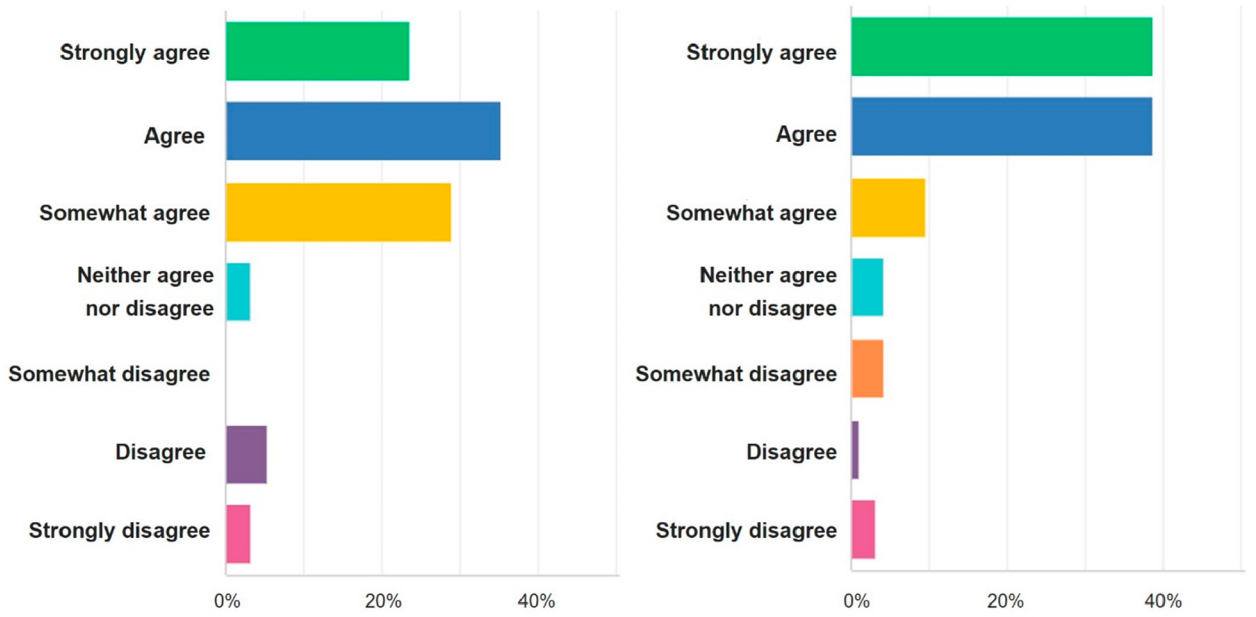

Figure 4. Response distribution for "MoleculAR helped my understanding of 3D shapes of molecules" (left) and "I found MoleculAR easy to use" (right). N = 123 (93 answered, 30 skipped).

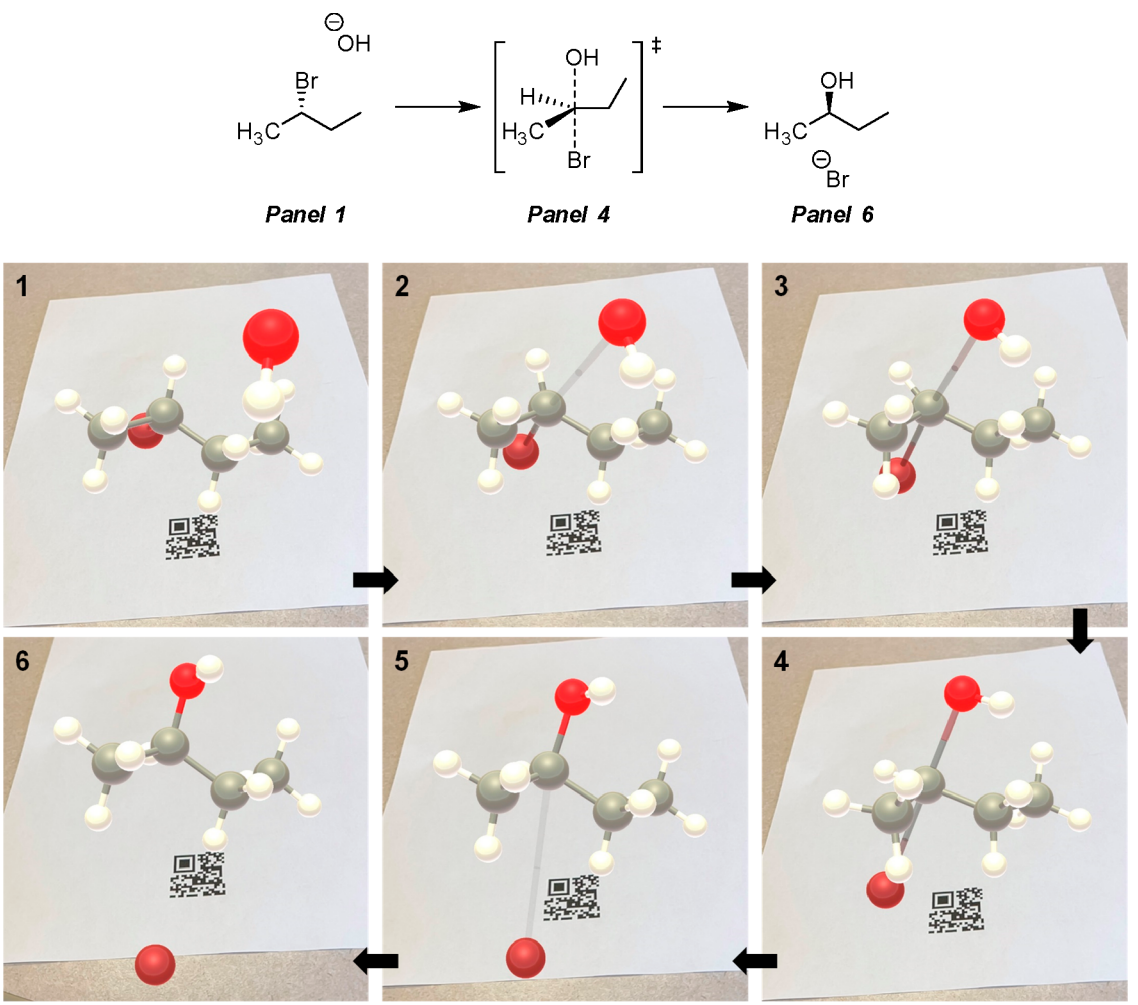

Figure 5. Six frames from a MoleculAR animation of an S_N2 reaction: a hydroxide nucleophile reacts with (*S*)-2-bromobutane to give (*R*)-2-butanol. The animation can be interacted with in the same way as a static 3D object.

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their agreement with two statements: "MoleculAR helped my understanding of 3D shapes of molecules" and "I found MoleculAR easy to use". The responses were overwhelmingly positive (Figure 4), with 88% of students agreeing that the app helped their understanding of 3D geometry and 87% agreeing that it was easy to use. These results indicate that the app was well received by students and that they perceived it as being helpful to their comprehension of 3D geometry.

Student Challenges and Addressing Barriers

The survey results showed that, while the majority of students who responded to the survey found the app helpful and easy to use, some had suggestions for further development. Specifically, students reported that the app was difficult to use for those who were visually impaired or for those who did not have access to a smartphone. Furthermore, some students had limited access to the app when working on older iPhones or Android devices, with compatibility limited to iOS 11.0 and Android 7.0 or later. These limitations and challenges were taken into account when planning future developments for the app.

Using the feedback from students and colleagues, we plan to implement new features to enhance the app's functionality and user experience, while maintaining simplicity of use. Some of the requested features are axis lines and nodal structure on orbitals; the ability to view bond angles and distances on the structures; and structure saving to a library with the names of molecules. The app's content has been expanded to include more complex orbitals, including *f* orbitals and molecular orbitals, and more complex molecules, such as biomolecules, natural products, and materials. In addition, we have started to add animations for dynamic processes like bond rotations and conformation changes as well as simple animations for bond breaking and making (see Figure 5 for an S_N2 substitution reaction). These features will enable the user to learn more about the structure and behavior of molecules and orbitals, as well as visualize chemical reactions.

Through all of these improvements and design iterations, a key priority has been to make the app accessible to all students, regardless of their background or access to technology. This was an initial limitation with the app's availability in the first year of trial, with some 15% of the CHEM 101 class missing out on this interactive experience as the app was only available for iPhones. To expand accessibility, the app has been made available for free download and use and is multiplatform, meaning that it can be used on both Android and iOS devices. Additionally, physical molecular models[24,26] have been made available in the classroom to visually impaired students or those who do not have access to a smartphone. The app is also used on an entirely voluntary basis in the classroom, and students can choose to use it in class or on their own time as they see fit.

CONCLUSIONS

MoleculAR is a functional cross-platform app built with user-centered design principles in mind, with the goal of creating an intuitive and user-friendly interface for learning 3D molecular geometry. By giving molecules a virtual body, the app supports learners to comprehend and predict molecular behavior, particularly those who have difficulty visualizing microscopic structures. The interactive graphics, with the ability to rotate and manipulate the virtual structures, create opportunities for learners to engage in conversations, explore different perspectives, and share insights, thus making the symbol-microscopic correspondence in Johnstone's triangle more obvious. These valuable conversations will draw on the diversity of student backgrounds and experiences to build a safe space where learning chemistry becomes less daunting.

Overall, the MoleculAR app is an effective tool for engaging students in introductory chemistry courses and has proven popular with both first- and second-year chemistry students. We intend to implement MoleculAR into more advanced chemistry courses with links to biology and biochemistry, given that the skills students develop with the help of the app are highly transferable to other topics or disciplines. We hope that other educators will adopt MoleculAR as well and take advantage of the freely accessible library of QR codes to incorporate MoleculAR into their teaching. We welcome any feedback regarding the adoption of the app by educators to facilitate their teaching and improve the learning outcomes of their students.

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Author Contributions

The MoleculAR project was conceptualized by J.S.M., who supervised J.L. and I.C.C. in its development. J.L. was responsible for software development and programming. I.C.C. was responsible for writing (first draft), visualization, and web development for the GitHub hosting site. J.S.M., V.I., and D.C.L. tested and implemented the app in the classroom. Student surveys were conducted by J.S.M. and V.I. All authors contributed to writing (reviews, edits) for the final draft.

Notes

The authors declare no competing financial interest.

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