Molecular Representation of Organic Compounds in Augmented Reality

Sanjana S, Shradha B Kaba, Dr. Gururaj Murtugudde

School of Computer Science and Engineering,
REVA University, Bengaluru.

Abstract.

Due to the molecules forming the compound molecule, the structure becomes large and complex, making it increasingly difficult for instructors to teach and students to comprehend visually. There are currently only a handful of resource to help students learn and understand chemistry concepts better. AR is a new technology and its popularity is growing rapidly, and chemists are slowly starting to investigate the benefits of using AR in education. Augmented reality augments elements of the world. Information about three-dimensional structures can be difficult to represent in two-dimensional space, despite the fact that augmented reality allows users to view 2D structures in 3D.

Keywords— Augmented reality, organic chemistry, molecular geometry, human computer interaction

1. INTRODUCTION

Organic chemistry is conceptually challenging since visualization of the structures of molecules is strenuous in a 2D space. Furthermore, as we discover more molecular reactions, and the molecules themselves grow complicated, understanding intricate details spans into three dimensional representations.

Chemists are asked to draw molecules in simplified ways to convey the geometry of complex compounds. An emerging technique is the inclusion of augmented reality technology into the teaching and learning process.

AR is a technique that superimposes computer-assisted contextual data onto the actual world, removing the need to rely on 2D representations of 3D structures. An instructor is no longer compelled to make arbitrary judgements about the best representation for achieving the learning goal. This project goes beyond conventional 2D constraints, thus offering users the direct control of understanding these structures, through interactive interfaces thus inculcating cognoscible learning abilities. The analysis of molecular structures of chemical compounds is a critical goal in teaching chemistry theory since the interpretations of physical and chemical parameters of the compounds are obtained. Using 3D models of molecules to explain theories improves clarity, leads to improved comprehension of organic compounds, geometrical, and interference mechanisms, as well as the forecasting of chemical reactions.

Systematic Literature Reviews have been conducted in recent years to comprehend the use of AR in the field of education, and have provided context regarding the advantages, drawbacks, and limitations. A few SLR elaborates on how AR can affect learning methodologies, while others had particular objectives, with research on how AR has evolved and upcoming trends in learning systems. Only a few studies outlined the specificities of Augmented Reality being used to represent organic compounds at molecular levels. This corresponded to a requirement to understand how AR can be potentially used to develop new advancements and directly impact traditional methods of teaching.

The ability to comprehend organic compounds comes from a detailed understanding of the atomicity and structural representation of these molecules. Since the structures are to be observed and studied at molecular levels, being reliant on technology that can aid in visualizing such elements is vital. With AR gaining momentum in terms of development and use since the year 2000, it became relevant to understand the types of AR devices available, how chemistry education can be leverages as well as the limitations associated with this research. These set the foundational guide on upcoming advancements in education-focused AR projects, forming new aspects for future improvements and how these studies can transform current methods of learning..

A. Objectives

Application goals: To motivate students` interest in chemistry. To be able to study while having pleasure and to believe that the knowledge they obtain is relevant and valuable. To ensure that the AR interface is compatible with the vast majority of mobile devices.

3D structures that can effectively help people understand molecule for increased interactivity and user-friendliness. Therefore, we are confident that this system will provide a unique type of object visualization that interacts with more realistic virtual models.

1. Our aim is to increase learners' interest in Chemistry.

2. To be able to learn while having fun and deem the knowledge they receive to be relevant and beneficial.

3. Develop AR interfaces compatible with mobile devices.

4. To add more features to the application allowing users to customize the model according to their needs, such as changing colour, brightness, etc.

B. 3D spatial thinking

Spatial thinking is the capability to remember and manipulate abstract visual images. In chemistry, spatial reasonings are mostly taught using 2D paper models or by using 3D computational models.

These models are meant to assist students understand chemistry by merging information from the macroscopic, microscopic, and symbolic domains. Augmented reality apps may use the camera on a smartphone to transform 2D paper-based chemical models into 3-D representations that the user may manipulate.

C. Pain-points

Due to the molecule's chemical structure and the combination of different molecules forming the compound molecule, the structure becomes large. As a result, it becomes more and more complex, and visualizing compounds becomes exponentially difficult.

When chemistry majors are often asked to draw molecules in a simplified way on a 2D interface. This may not be effective in understanding the actual structure of these molecules, otherwise understanding the chemical reactions of these molecules is very difficult.

Given the problems described above, it becomes clear why the development of a smartphone application to visualize molecules in three-dimensional interface will be beneficial. This reduces discrepancies in understanding organic chemistry and encourages others to understand comprehensive topics easily through their own pace.

2. PROBLEM DEFINITION

"How might we develop an AR Application which encourages, aids and motivates students to visualize molecules to enhance their understanding of molecular chemistry "

The challenge of visualizing molecules in 3D arises in the chemical sciences at many levels, from teaching the concepts of stereochemistry to visualizing the complex molecular structures. As molecules get bigger, more complex, and expand into three-dimensional space, visualization becomes more and more difficult. Chemists or teachers often need to draw molecules in a simplified way to represent the geometry and symmetry of complex compounds. A simple way to visualize molecules in 3D would be very helpful.

3. MOTIVATION

The motivation towards developing this project is focused towards aiming to advance conventional learning methods being used to teach students, towards a futuristic approach that can leverage AR to better educate within the scope of molecular chemistry. The scientific motivation can be attributed to encouraging users to involve themselves with the activities, conduct experiments and review their findings.

Primary, the scientific motivation towards this study can be attributed to four influential factors: encouragement to learn science and explore its sub-branches; intrinsic motivation- to create a self-assessed understandings and findings from experimental data; and self-efficacy. The ability to leverage AR through these findings, to create an advanced learning environment that is accessible, easy to understand chemical concepts at a molecular level, and can be improved is the primary motivation that led to the development and research of this project.

4. AUGMENTED REALITY

Consider Virtual Reality to be an umbrella term, this term constitutes other findings such as augmented or mixed reality. Unlike conventional Virtual Reality, Augmented Reality has a user interface that integrates the physical and virtual worlds, enabling consumers to combine real-life surroundings with virtual objects for a native and pragmatic experience. AR enables the interactive and real-time merging allowing users to see the information they perceive, in reality.

It's worth noting that Milgram and Kishino's definition focuses solely on graphic representation. However, in this instance, AR might be regarded as a bridge between virtual and real-world perspectives, with AR acting as a supplement to VR. As a result, Augmented Reality cannot totally reinstate the physical universe; rather, it gives us the impression that simulated and physical items co-occur in the same space. Azuma study, otherwise, recommends three important features for computational systems that embrace AR:

(i) blend simulated elements with the actual world; (ii) are interactable and enable real time processing the key concept driving the usage of AR in such research is the creation of immersive digital materials and technologies that provide consumers with unique & effects.

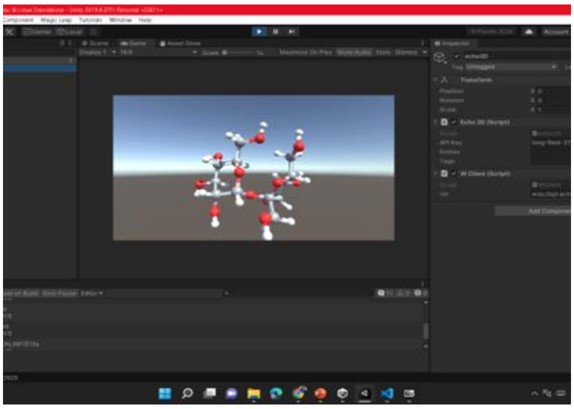

Fig 1: Unity app for building AR scenes

5. LITERATURE SURVEY

D. Eriksen, Nielsen, and Pittelkow's (2020)

It can be challenging to present information on 3D structures in 2D, whether in compound or molecular form, for example, through textbooks or a digital device. Furthermore, augmented reality may be utilized to depict 2D structures in 3D and make the models user-interactive so that they are easier to recall and absorb visually for the peers.

E. Derek Behmke, David Kerven, Robert Lutz, Julia Paredes (2018)

Chemistry in Augmented Reality: Creating Interactive 3D Structures from 2D figures made possible, according to research on visual spatial capabilities in chemistry, it was discovered that students struggle with comprehension with molecules owing to their complicated architecture and incomplete design, making it tougher to make sense of it. As a result, blending AR into learning can dramatically boost learners' capacity to interpret.

F. McCormack (2014)

Augmented reality- invent. Through the research it was observed students had to deal with great difficulty with chemistry, particularly organic chemistry. To address this issue and to test the effectiveness of AR technology, Fresh college chemistry students were prepared for online teaching in a virtual lab. After a month of study as a result, most learners say this is a great tool and will recommend it to others. While many VR applications have proved useful, interactive VR techniques are thought to be challenging and limiting.

G. Barak, M. (2013)

Making Visible: Integrating 3D Molecular Imaging into K-12 and Post-Secondary Education Even at the college level, many students struggle with three-dimensional visualization. These issues stem from a misunderstanding of fundamental chemical principles. AR technology, on the other hand, may be utilized in institutions to help students establish a better foundation and make studying an enjoyable and productive process through interactive engagements.

6. DISCUSSION AND RESULTS

On conducting further studies into Valence Shell Electron Pair Repulsion – a defined principle that explains how chemical structures are. The geometrical structure of the molecules can be explained using this theorem, which can calibrate the intensity of electro-static repulsion for better understanding. Furthermore, we can leverage these findings to make an educated guess about the shape and structures of said structures. Through trials and tribulations, it has been established that one tends to interpret special objects and gain a better understanding when they can view them in three-dimensional spaces. Thus, it is encouraged to push this forward thinking methodology through practice. For instance, three-dimensional printing and simulation experiments are popular models.

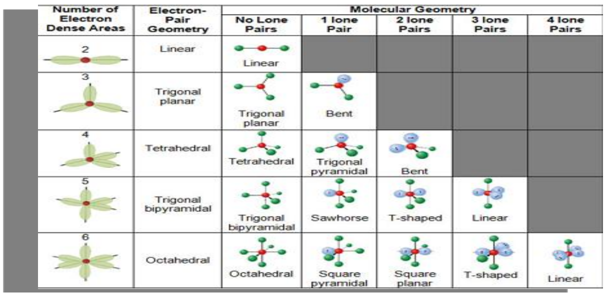

Fig 2: VSPR in theory

When a smartphone is pointed towards a flat surface, a 3D model appears, which may be modified in many ways (inversion, magnification, seeing from various angles) to better comprehend its structure and operation. The applications that have been posted make it possible to create the study content and make it simpler to remember. The instructor, on the other hand, has the capacity to shorten the time it takes to explain a theory and to use that time to address contentious issues, solve creative problems, and so on.

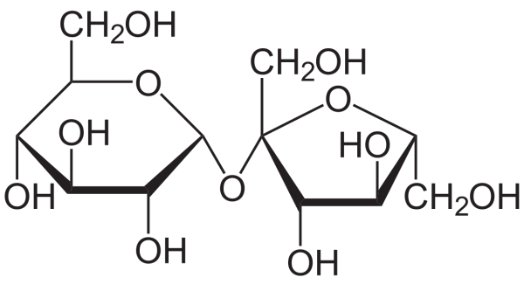

Fig 3: Chemical structure of a Sucrose molecule

When the chemical structure of Sucrose is illustrated in a two-dimensional interface, it is evident that the structure is difficult to comprehend. The molecules are arranged in a 3D format and viewing them on a plane surface can be cumbersome to understand and interpret. Using our AR application, users can now view these molecules in an augmented reality environment, and can interact with these structures, by moving them and observing the chemical composition in a comprehensive way that also makes it easier to remember.

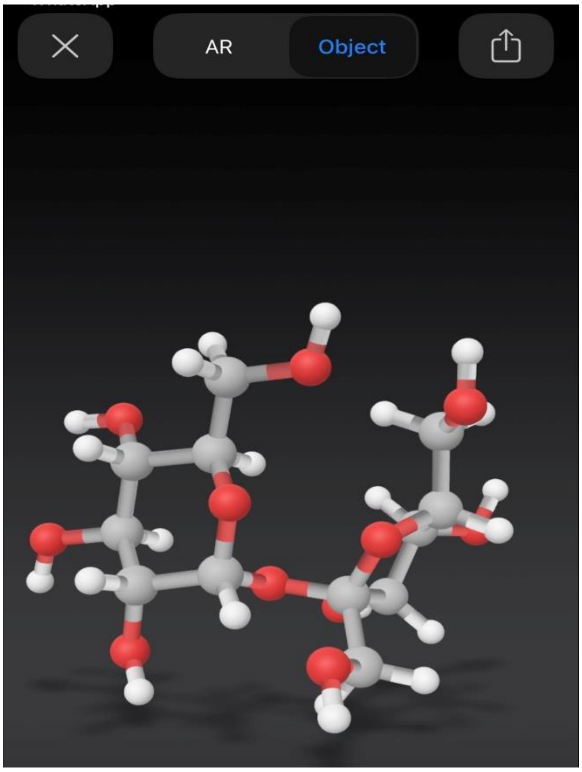

Fig 4: Sucrose molecule in an augmented reality environment

This is a research and development project that follows a scrum-agile methodology, research, design, development, implementation, and review are the five steps of the workflow.

When it came to research, we decided to distribute a questionnaire that contained questions pertaining about Augmented Reality and topics pertaining to chemistry. Furthermore, we reached out to students who were willing to share their opinions about understanding molecular concepts and their experience with using augmented reality. This exercise gave us much insight into understanding the general expectations one may have when it came to sing educational apps, and the use of apps that are accessibility friendly and is engaging as well.

In summary, these insights provided details into what students expect when it comes to being able to integrate AR apps with a better understanding of chemistry. With over 91.4% being interested in using AR apps for better understanding of stereochemistry; over

78.23% having prior knowledge of using AR apps and 67.40% answering affirmitavely when questioned if learning chemistry would be better comprehendible in an interactive environment. These are a few instances of the data that was collected.

With this information, we proceeded to the design phase of our application. Here, we wanted to initially establish requirements that were fundamental and then proceeded to conduct sprint reviews of the workflows, user interface components and colour scheme that was in relation to the overall theme. The tools we used here, were Figma, Notion and Dribbble.

When it came to development, we had a deep dive into the various available tools in the market and which one closely resembled our interests. This includes understanding the popular software, verifying their usability, open source friendly as well as the overall development time required.

This introduced us to tools such as Unity, Vuforia, AR Kit etc. Here, we also had to make trade-offs between usability, costa as well as development platforms. With us focusing on developing on Android devices first. This phase was about understanding the components that were required, such as AR physical tools, 8chemical structures that can be viewed in a three-dimensional plane of view and an APK that will be able to install on devices for further testing. Overall, the major software used were:

- Unity 3D
- Vuforia
- Android Smartphones
- JMol

Ultimately, we wanted to be able to test our application. Besides the failure mechanisms that we had in place through the device's code, we also conducted a test on various Android versions to verify background compatibility. We also were able to test it among a group of students and teachers, primarily from chemistry backgrounds and collected feedback for improvable features in future iterations. Finally, we verified the usability of the application by collecting end user data.

7. COST ESTIMATION

When discussing Virtual Reality, the clientele is large, and it continues to grow. Companies like Facebook, Google and Amazon have released software that inculcate the use of virtual reality and the trend is also spreading towards augmented reality and mixed reality domains.

In VR markets alone, the users have crossed over a billion, and the revenue overall has been trifold in recent years. The user curve is only expected to go higher, with predicted values in billions by the end of the decade.

Additionally, the technologies have not only reinvented the concept of gaming, learning, and have started to increase in other industries, they have also become more accessible. This encourages growth and aids many groups to enjoy augmented reality developments, while also using them independently.

With this technology booming as of late, the overall costs of developing an app for augmented reality ideas becomes an important decision. Like any other software, the costs are dependent on several factors ranging from active clientele to geographic locations. The convergence of the physical world with augmented virtual experiences is an emerging study. With these in mind, some factors that influence the development of an AR app are as follows:

1. Software – The software used for an application is a huge element that influences costs. This is due to the multitude of software available on the market, choices between open-source or licensed software and also, development platforms

2. Development Time – This can range widely but it is acceptable to estimate an average time of 150-180 hours.

3. Features – Augmented reality can be simple or have advanced features. Understanding your app requirements is vital to estimating the features required in an AR app, and furthermore, concluding quality and costs associated with it.

In a recent article, there were a few other factors highlighted that can determine the costs involved in the development of an AR app. These were, based on location, slam or marker apps. However, the biggest cost estimator is based on the device software as well as external devices such a VR headset and handheld devices.

8. Compliance with Society

The tremendous advancements in AR in the realm of education, and particularly, have spurred a rapid development of its utilization in learning and teaching operations. AR has prompted a great deal of interest in the discipline of chemistry, primarily because it allows students to comprehend processes that aren`t apparent to the unaided eye.

We have also complied with accessibility principles, in order to improve our application and make it convenient, thus enabling these decisions in order for everyone to take part independently. The importance of accessibility was a study conducted by Texas State University, it emphasizes access by everyone, regardless of disability is an essential aspect.

To overcome: teaching approaches are still focused on fact retention. Information is frequently tough to grasp, there is a lack of involvement.

9. Conclusion

The extraordinary growth of AR in the field of education, particularly in the field of learning and teaching activities, has driven the rapid development of AR usage in learning and teaching activities. AR has sparked attention in the realm of education, primarily because technology helps pupils to comprehend processes that are invisible to the human eye.

AR has been incorporated with many educational experiences ranging from Google Expeditions (a hybrid of AR and VR that spotlights notable sights and artefacts) to Geo-Goggle, which teaches how to measure altitude and distance between two points using a 3D compass.

The current method of learning presents substantial challenges: The pedagogical method is still centred on knowledge retention. It has been observed that information is frequently descriptive. In and out of class, there is a lack of participation.

Making the student experience more pleasurable is one of our answers. Virtualized in order to improve interactive comprehension and learning. Improves student engagement, comprehension of complicated topics, and personalised instruction, increases learning retention, and reduces reliance on learning by rote.

However, using AR and VR in eLearning can be costly since these technologies require pricey software and gear. AR and VR both require a lot of room and restricts mobility.

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Biographies

Photograph

Author Name received the bachelor's degree in computer engineering from Cankaya University in 2010, the master's degree in computer engineering from Gazi University in 2014, and the philosophy of doctorate degree in Electrical-Electronics & Computer Engineering from Duzce University in 2017, respectively. He is currently working as an Assistant Professor at the Department of Computer Engineering, Faculty of Engineering, Duzce University. His research areas include mobile security, deep learning, and social network analysis. He has been serving as a reviewer for many highly-respected journals.