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From Plastic Models to Virtual Reality Headsets: Enhancing Molecular Structure Education for Undergraduate Students

Chaleena Pimpasri[a] and Taweetham Limpanuparb*[a,b]

Abstract: The comprehension of molecular structure is pivotal in chemistry education. Over the past decade, Mahidol University International College has employed various teaching tools for the introductory chemistry laboratory class. This paper outlines our evolutionary shift from traditional tools, such as plastic and plasticine models, to the integration of computer software, and ultimately to augmented reality (AR) and virtual reality (VR) tools—specifically, MoleculARweb and MolecularWebXR developed by École Polytechnique Fédérale de Lausanne researchers. In this paper, we detail the implementation of these tools in our classes and present the outcomes of student surveys. Our instructional focus encompasses VSEPR, Atomic Orbitals, Molecular Orbitals, Skeletal Formula, and Enantiomers. This paper not only serves as a model for educators in general chemistry at secondary school or university levels to incorporate technology into their classrooms but also showcases a collaborative endeavor between Swiss and Thai researchers.

Keywords: Chemistry education · Molecular modelling · MolecularWebXR · Virtual reality

Dr. Chaleena Pimpasri is a new lecturer of Chemistry at Mahidol University International College. She recently graduated from Imperial College London under the supervision of Dr Silvia Diez-Gonzalez in August 2023. Her research interest includes synthetic methodology and catalysis. She is currently the course coordinator for introductory chemistry laboratory.

Dr. Taweetham Limpanuparb is an Associate Professor of Theoretical Chemistry. He is a recipient of the Thailand's Young Scientist Award (2020). He earned his PhD in Quantum Chemistry from the Australian National University (2012). His research interests include theoretical/physical chemistry, computational/multidisciplinary science and science education/communication.

1. Introduction

Phankingthongkum and Limpanuparb[1] systematically reviewed more than 40 literature articles on molecular model teaching tools up to the year 2020 and discussed repurposing two open-source molecular graphic software tools from a relatively specialized use by researchers in related fields to a general use by natural science undergraduate students studying general chemistry. In this introduction, we revisit the teaching practice before 2020 at Mahidol University International College (MUIC) and how the interaction with the researchers at École Polytechnique Fédérale de Lausanne (EPFL) has inspired changes in the way we deliver the molecular structure laboratory to general chemistry students.

Fig. 1 shows the timeline of introduction and evolution of 'molecular model' practices[2-4] in MUIC chemistry laboratories. Before 2016, the class only covered traditional wet experiments. The second author (TL) introduced a series of changes to incorporate theoretical and computation aspects of chemistry to each of the experiments. One practice that was introduced as a standalone non-wet lab is molecular modelling. Available literature at the time was consulted and followed. The lab was considered a special experiment and was revised every trimester in search of an optimal protocol for the class until 2019. After a series of changes and improvements in the middle of the COVID-19 pandemic, we have settled for our own version of the molecular structure laboratory implemented on open-source software (Avogadro and IQmol). This was designed with the main aim to develop spatial thinking skills through interactive teaching tools[5-7] and was published in 2021.[1]

Our interaction with EPFL team occurred after the publication of the paper on the use of software. We learned of MoleculARweb, a free web service that can do almost the same tasks as can be done on the open-source software without the need for software installation on a computer.[8] We quickly embraced this AR tool for teaching[9–10] which happened under physical distancing during the pandemic period. Students used MoleculARweb from their mobile devices in addition to the university computers and this was a hygiene advantage when class gradually returned to campus with restrictions. We updated the addition of the browser-based approach in the online manual[9] and social media[10] but have not reported it in the literature.

In 2023, the EPFL team invited us to test their new evolution from MoleculARweb to MolecularWebXR.[11–13] The new VR delivery approach is still web-based but, rather than using existing hardware (smartphone/computer) and paper AR markers, a new set of hardware (VR headset) was required. Modifications to materials are also needed for the implementation of VR technology. Our work on the integration of MolecularWebXR into a classroom practice is therefore the main focus of this paper.

*Correspondence: Prof. T. Limpanuparb, E-mail: taweetham.lim@mahidol.edu

[a]Mahidol University International College, Mahidol University, Salaya, Phutthamonthon, Nakhon Pathom 73170, Thailand; [b]School of Chemistry, UNSW Sydney, Kensington, NSW 2052, Australia

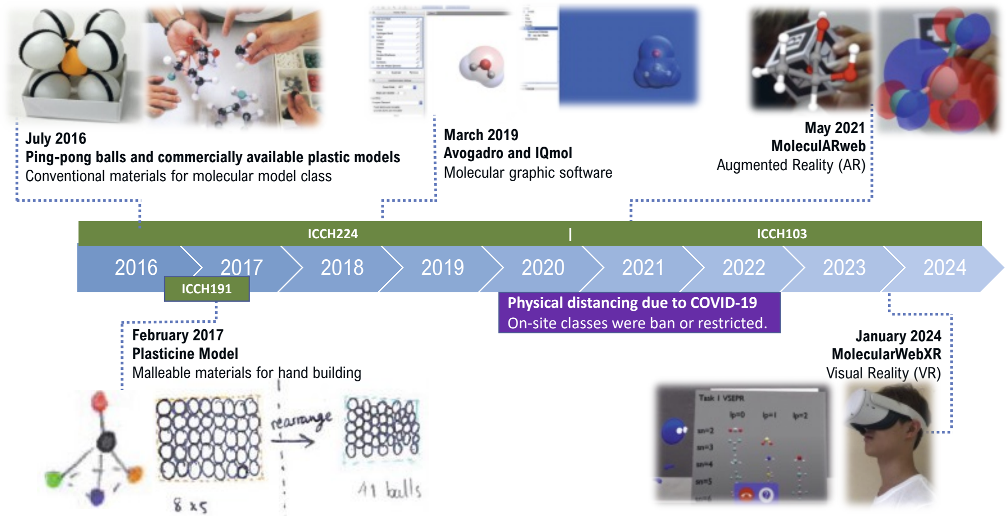

Fig. 1. Teaching medium and/or technology platform for molecular model teaching implemented at Mahidol University International College. ICCH103, ICCH191 and ICCH224 are laboratory courses to accompany general chemistry class for science and dentistry students.
Top left image was reprinted (adapted) with permission from *J. Chem. Educ*. **2017**, *94*, 827. © **2017** American Chemical Society.
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2. VR Environment Preparation

In the past few years, the shift in the development of modern tools for STEM (Science, Technology, Engineering, Mathematics) education transitioned from traditional software for modeling and molecular graphics to augmented reality (AR) and virtual reality (VR). AR/VR tools offer users 3D structure visualization, making the comparison and manipulation of two molecules more straightforward than working with 2D structures on a flat screen. AR tools allow users to see virtual molecules overlaid onto the physical world. In contrast, VR tools provide users with a fully virtual environment.

MolecularWebXR is one of the free-to-use platforms that specializes in immersive VR tools for interactive learning. The website not only provides real-time discussions with preset 3D materials but is also compatible with basic devices operated with VR headsets. The developer also provides users with an empty room to load their own pre-built objects. Affordable VR headsets, with a price less than 300USD (~10,000THB or ~250CHF) for Meta Quest 2 (previously known as Oculus Quest II),[14] along with another device (preferably, a desktop or laptop computer) connected to the internet on the same network, offers immersive visual experiences. While the VR headset is Android-based but as the name 'WebXR'[15] suggests, the service is entirely web-based and app-free enabling users to use it instantly with a standard browser on their platforms. This trend of returning from App to Web is consistent with recent chemical education literature.[16,17]

Preparations for the VR environment, physical space, hardware as well as changes to the lesson plan are needed to implement this new technology in the classroom.

An empty room of the MolecularWebXR was used here. Therefore, 3D objects must be manually prepared in advance for the exercise. These objects are mainly hand-drawn molecules but also include text labels and orbitals. The preparation can be done in a verity of open-source software (*e.g.* Blender[17]) in a similar way to preparation of 3D printing models, which we have earlier incorporated into the laboratory class.[18-20]

Fig. 2 provides the technical pipelines of how different types of files are converted. The final products are *.glTF* files hosted on EPFL site. For security reasons, users are not allowed to upload *.glTF* or provide an external URL directly. This *.glTF* was produced *via* an upload of either wavefront (*.obj* & *.mtl*) or PDB files to PDB2AR site.[13] The preparation is only needed once and the files (as links) can be kept for future use.

For the person wearing the VR headset to walk safely, the class must be relocated from the traditional chemistry laboratory to a suitable environment. Quiet public indoor open areas were initially used without prior booking. (VR headset is not recommended to be operated in an outdoor setting.) Later, either dance or yoga rooms were booked for this purpose. The rooms are empty, air-conditioned, and equipped with one computer, LCD projector as well as a whiteboard and a mirror wall. This setup allowed one person to wear the headset and the rest of the class watched the demonstration activity through a 'second person perspective' from the screen of the projector. (The alternative is to use the casting feature of the VR headset to give a 'first person perspective' of the room.)

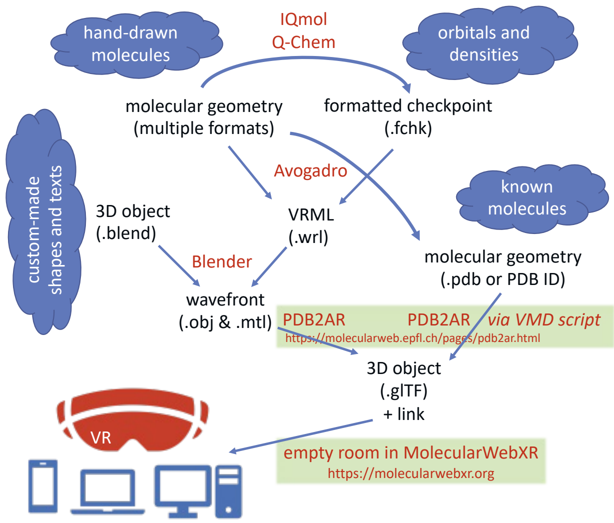

Fig. 2. Technical development pipeline for implementation of MolecularWebXR in molecular model.

In this setup, at least two operators were needed. The main control of the virtual room (loading, deleting, resizing, and locking objects) was from the computer. A free browser plug-in on the computer was used to record the screen. Students used the recordings to complete the worksheet after the demonstration. The manipulation (moving and resizing) of objects after loading was done by two wireless hand controllers as part of the headset.

For the class of ~20 students, it is impractical for all to wear the goggles concurrently in the same room. At this time, while the technology is relatively inexpensive, it is still new and requires proper induction and supervision to ensure safe and effective use. The short-term solution is for the instructor to lead the class for approximately one hour. After the demonstration, students were allowed to individually interact with the device under one-on-one supervision by the instructor on a time-sharing basis for another hour. This is the optimum use of one device with the battery time of approximately two hours.

3. Pedagogical Approach

For Trimester 2/2023-24, there were two sections of the introductory chemistry laboratory class for undergraduate students, comprising of mostly first- and second-year students at MUIC. Forty students were randomly assigned to work in pairs, tasked with completing a two-page worksheet within a four-hour laboratory session. The VR activities took place in a dance room, offering ample space for the person operating the headset, and the groupwork on the worksheet was completed in a computer laboratory. Worksheet and study materials on related topics were given to the student one week before the class.

On the day of the class, the instructor led the activity by manipulating objects using the VR headset and giving verbal explanation simultaneously. (Voice communication feature of MolecularWebXR was not used as the instructor team and students were all in the same room.) The demonstrations were shown on the LCD projector with the assistance of a second person who operated the computer as a camera person and recorded video clips or captured the screen as needed.

Inspired by more recent (from 2020) educational literature on VR,[21] digital interactive media,[22] metaphors on formation of molecules from atoms,[23] visuospatial thinking[24] and neuropedagogy,[25,26] our original four tasks from 2020[1,9–10] were revised and expanded into the following.

The pre-lab briefing began with a pre-activity questionnaire assessing their understanding of fundamental concepts in stereochemistry, as well as their expectations regarding the integration of virtual reality in chemistry education. Then, we discussed the stories of Kekulé and van't Hoff and their roles in molecular structure theory. The famous but rather old anecdote of snake and benzene and the connections from the two scientists to the students by *academictree.org* were presented before introducing VR, a relatively modern technology to the class. Five tasks below were presented by order of difficulty and reflected the order of topics taught in general chemistry and organic chemistry. As the audience was mainly science students from non-chemistry majors, biomedical science-related examples were given more consideration in these tasks.

In **Task 1**, the instructor illustrated a set of representative molecules according to the Valence Shell Electron Pair Repulsion (VSEPR) theory. This demonstration incorporated two considerations (steric number and number of lone pairs) on the molecular geometries (*e.g.* trigonal planar, tetrahedral, and square pyramidal). The immersive VR experience empowered users to control the size, orientation, and position of the molecules.

Task 2 involved the visualization of atomic orbitals from hydrogen atom. Students appreciated different shapes of s, p, and d orbitals. The relative energy levels and shapes of orbitals are important basics to understand electrons in atoms and molecules.

Task 3 demonstrated molecular orbitals (MO), specifically the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of reactants BH_3 and NH_3. This task aimed to deepen the understanding of the formation of the BNH_6 product according to Lewis's acid-base concept.

Task 4 introduced various bond-line structures (*e.g.* wedge-and-dash, Fischer, Newman, and Haworth projections) in the students' worksheet. During the demonstration, students individually matched these 2D structures with their corresponding 3D representations, facilitating a comprehensive comparison of similar structures simultaneously.

In the bonus task, the demonstration focused on two pairs of well-known enantiomers, thalidomide[27] and carvone. The term 'superimposable' and 'mirror image' were discussed and demonstrated through VR. To provide a tangible and multisensory experience, students also smelled two samples of the *R* and *S* stereoisomers of carvone[28,29] as a direct observation of enantiomeric effect. This is in line with a 2023 study using smell combined with VR in the lesson of French lavender production.[25]

At the end of instructor demonstration for the whole class, the student moved to the computer room to write a report on their findings of the five tasks. They worked in pairs and used video clips and screen capture from the VR room to fill the worksheet.

The time schedule for this individual interaction was communicated to students before they moved to the computer room. During their appointment time, each student also had a 3-minute opportunity to operate the VR goggles before proceeding to an olfaction blind test to identify carvone enantiomers. (The two compounds were obtained from Tokyo Chemical Industry and used without further purification. Their purity and enantiomeric purity claimed by the manufacturer are ≥ 98% and ≥ 96% respectively by gas chromatography.) A procedure by the Royal Society of Chemistry suggests that it is a relatively safe experiment when the student smells the compounds from a bottle containing a ball of cotton wool and ten drops of the enantiomer.[28] Hence, gloves and eye protection were not required and this was conducted outside the laboratory setting. Students were given the explanation that the *R*-(-)-carvone (also designated by relative configuration L-) is found in spearmint while the *S*-(+)-carvone (or D-) is found in caraway. Students are encouraged to identify them by smell through a double-blind test of four samples.

Pre- and post-activity questionnaires were administered, conducted on 26 January 2024, within this laboratory period immediately before and after the activity. The study was approved by Mahidol University's IPSR-IRB, certificate of approval no. 2020/05-241. Written informed consent was obtained from all participants. Student interactions with the VR headset and test of smell of carvone were voluntary under the one-on-one supervision of the instructor. AR activity on MoleculARweb and plastic models of carvones were kept as alternatives, should any student declines the interactions.

Fig. 3 shows a sample of the results from the five tasks completed by taking snapshots of videos recorded from the MolecularWebXR.org. The class time and quality of the reports are comparable to results produced earlier by other tools.[1,9] Students were excited to be the first in Thailand to experience this emerging educational technology. In free-listing section of the post activity survey, they reported comments such as 'really fun', 'good time' and 'want to play again'.

Our main focus of the survey was students' familiarity, expectation and acceptance of the technology as the information would help instructors make a decision to introduce/adopt VR into their teaching. With a limited number of participants ($n = 40$), preliminary findings presented below may be regarded as a trend and may not extend to a larger population.

Pre-activity: While most of our students had heard of VR but had not yet tried it prior to the class (47.5%) or tried it at least once but do not use it regularly (42.5%), the majority of them have the right expectation that VR in class will be used to manipulate molecular models' size, location and orientation in 3D space (70%).

Post-activity: On the matter of cost and distraction, the majority of students agreed that VR is relatively affordable (85%), is not a distraction in classroom (80%) and is useful for education (95%). In terms of institutional support, students ranked VR headset as the third priority after laptop/tablet and 3D printer/scanner and before two subscription services.

Two questions in the post-activity survey are similar to a 2023 report from UCLA ($n = 12$).[17] Students in current study had higher prior exposure to the 3D/AR technology (Fisher's exact test p-value <0.05) but their wish to see more of the technology in future classes is similar (χ^2 test of homogeneity p-value=0.149).

VR motion sickness: In a free comment section of the pre-activity survey, two students reported their concern about VR motion sickness. In the post-activity survey, students disagreed that they have any discomfort in using VR (85%).

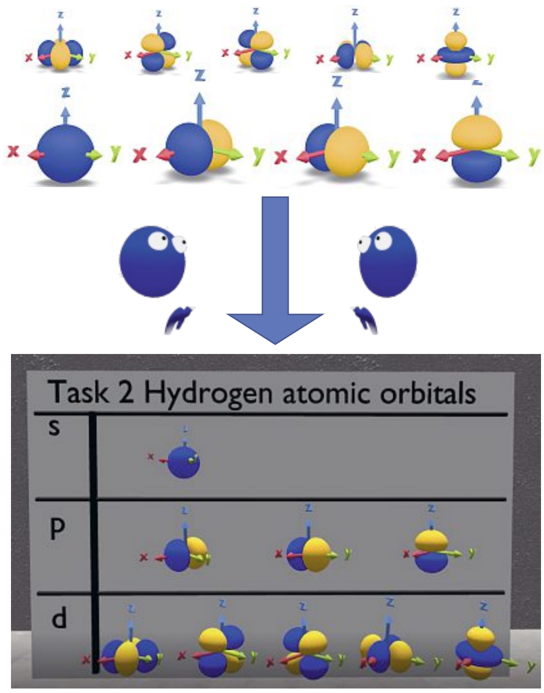

Fig. 3. Atomic orbitals cannot be reproduced by plastic models but are available in the software and AR/VR tools. Top: individual 3D objects of s, p and d orbitals. Bottom: A MolecularWebXR screenshot after 3D objects were imported and arranged.

For more information, the supplementary material contains instructor notes, student worksheet (blank and solution), questionnaire forms (blank, tallies and further thoughts on inconclusive points such as olfactory test) and video/screen recordings of the tasks described in this paper.

4. Concluding Remarks

We demonstrated that MolecularWebXR.org can be adopted for chemistry classroom teaching with a minimum investment of just one VR headset. Existing teaching methods and materials have been revised and evaluated with this new immersive environment. Improved student experience suggests that this new implementation can also be readily adopted elsewhere to meet emerging expectations from learners. Olfactory activity as part of multisensory learning activity in chemical science also warrants further investigation in a separate study.

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Author Contributions

The two authors contributed equally to this paper. The authors declare no conflicts of interest. The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript.

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