

Can Virtual Reality Increases Students Interest in Computational Chemistry Course? A Review

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Abstract

Computational chemistry is one of the branches in chemistry that implies the finding of theoretical chemistry into efficient computer programming to monitor, calculate and examine the properties of molecules and solids, adopting these programs to real chemical problems. Intersection between virtual reality (VR) and computational chemistry would bring the strength and improve the weakness of the system for better chemistry field discovery among scholars that level up the educational development. Thus, introduction of VR as an educational medium will eventually add another new technical skill for good purpose mainly for processing data and information. This paper reviews the role of VR as a teaching device in computational chemistry courses. The innovation in teaching and learning helps students to collect more reliable and quality data on the chemical analysis that is not available from the experimental works. This will provide source and bridge for the students to easily collect and analyse data in comprehensive understanding especially deep explanation at atomic level. This teaching strategy also stimulate and attract the interest of the students to be more joyful and native in learning.

Keywords: Virtual Reality; Computer Simulation; Computational Chemistry; Undergraduate; Molecular Dynamics; Laboratory Computing

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INTRODUCTION

An education in chemistry offers a scientific perspective on the makeup, structure, and characteristics of matter, as well as the transformations that may take place in matters. The major objective of chemistry education at the undergraduate level is to provide students with the ability to explain macroscopic occurrences based on a microscopic perspective of the subject matter (Chakraborty & Maity, 2020; Chirikov et al., 2020). Analysis of chemical structures and how those structures change over a range of thermodynamic states is a significant focus in today's chemistry classrooms. Even so, observing the changes in complex molecules is quite challenging, especially when relating conceptual and theories about the actual mechanism in molecular structure that occurred in real life. (Radianti et al., 2020).

There is no denying that the awareness and exposure in the field of theoretical chemistry has been welcomed and achieved by excellent progress through the formation and development of chemical modelling that covers a wide and different field. This is proven when computational chemistry received the Nobel Prize in

Chemistry in 2013 (Schlick, 2013) and can be a strong support for the suggestion to introduce computational chemistry courses among undergraduate students. The main modules contained in the computational chemistry such as molecular dynamics (MD) simulations (Rapaport, 2014), reaction kinetics simulations (Cruz et al., 2020) and quantum mechanics (QM) calculations (Agnesi et al., 2018), can be considered as the part of subject courses. Among those examples, MD method will be the suitable and convenience method to apply for the beginner especially for the students. From there, students will be introduced and be able to explore the molecular dynamics at atomic level that involve the movement of atoms and the process of how they are being interacted together. Yet some issues are not really resolved as both visualization and modelling are come in different way and do not synchronize to the single approach. Therefore, students are required to conduct some steps of simulations to obtain the output file before they can proceed to the molecular visualization. At this stage, there is lacking in device selection for the visualization especially for the use in classroom since some of them are not coming with good expertise or even being outdated from the current technology.

Virtual reality (VR) has advanced quickly over the past ten years due to advancements in visualisation technology, reaching a point where it is ready for use in classroom (Luckerson, 2014). Virtual reality presents a fresh possibility for education and may completely alter how modern courses are taught. Virtual worlds are built through the visualisation of VR technology to enable real-time, multimodal interactions between users and the intended system (Cipresso et al., 2016; Di Lernia et al., 2018; Freeman et al., 2017; Neri et al., 2017; Riva, 2018). A new age in chemistry education has recently begun with the use of VR, which offers 3D spatial resolution and flexible molecular structure manipulation (Feiner et al., 1997; Schmidt et al., 2017). An excellent instructional application was created by the interactive MD in VR (iMD-VR), which was first propelled by DFTB+ code, employing a modest reactive system (Deeks et al., 2020). Some might find that it is quite impossible to implement those application in chemistry field. However, it is actually doable and reachable to achieve in any science fields. For an example, Ferrell and his team members implemented iMD-VR software as teaching medium in organic chemistry subject in order to improve the study quality (Ferrell et al., 2019). VR commonly come with some mechanical kits such as gauntlets and controllers that help the users to feel and explore the virtual visualization where in this case, the virtual environment of the molecules. From there, the user can actually immerse themselves into the environment by some sort of practical actions like "touching" and "dragging" molecular structures using controllers. Figure 1 shows the VR immersive visualization by participant that equipped with the headsets and hand controllers. Participants can simultaneously take a 360-degree tour of the virtual area thanks to the head-mounted display. This actually bringing some joys to observe rather than screen touching or mouse clicking on the computer monitor. All of this is actually achievable due to the advancement of technology from the VR itself (Pastel et al., 2022).

METHOD

The base of this review is extracted from the perspective of VR roles and impacts on the students' performance in learning such as self-attention, delivery, conceptual and confidence. One of the main sources in information gathering is Web of Science (WoS) under Clarivate Analytics. This platform holds an integrative fields of Journal

Citation Report (JCR) index where it filters all top standard journal reviews and arrange them based on the fields and topics. This making us easy to access and gather all the information across the worlds digitally by searching and downloading the possible reports including conference papers, book section and journal articles. The searching was done using keywords of "Virtual Reality", "Computational" and "Chemistry". The searching is beyond expectation where the result gives out a high number of related documents close to 1000 findings. Those results were narrowed down into specific fields, only related to VR to avoid the abundances of unrelated topic. Until 2018, more than 282 related articles were found that related to VR study (Goddard et al., 2018). This number is actually concluding the number searching for this review where more 200 documents including journal articles was found based on the keywords and case study.

RESULTS AND DISCUSSION

Virtual Reality for Teaching and Learning

Computational chemistry is one of the branches in chemistry that implies the finding of theoretical chemistry into efficient computer programming to monitor, calculate and examine the properties of molecules and solids, adopting these programs to real chemical problems. Intersection between machine learning (ML) and computational chemistry would bring the strength and improve the weakness of the system for better chemistry field discovery among scholars that level up the educational development. Recent study done by Keith et al. (2021) showed the needs of this corporation due to some issues and concerns such as inadequate technical expertise for comprehensive data collection, testing, analysis, and validation.

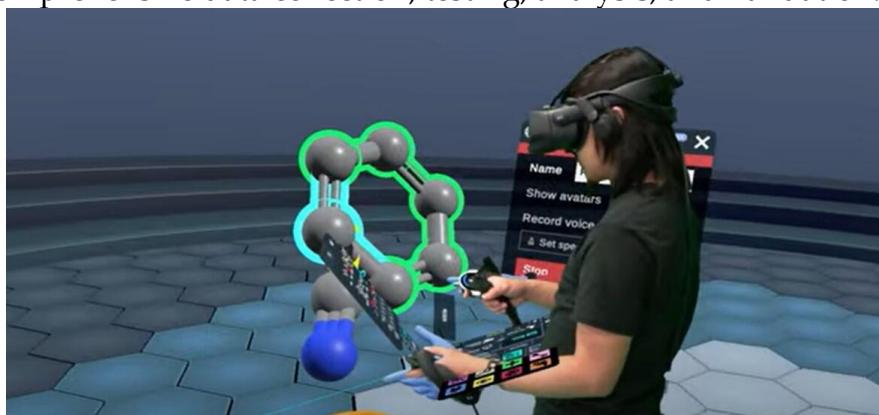


Figure 1: Snapshot of VR immersive visualization for molecular building. Participant is equipped with headsets and hand controllers for visualization control. Picture was obtained from Nanome, Inc. Nanome: Creating Powerful, Collaborative, and Scientific VR Tools. San Diego, CA, (Nanome, 2022).

There is no doubt that VR plays an important role in student learning (Fombona et al., 2020). However, it is still an issue when there are not enough records about the effects of VR on student learning. This is explained when the assessment of learning through laboratory practice and VR does not produce a significant impact on each other (Dunnagan et al., 2019). The lack of research and studies on VR applications is likely to be the reason for this even though VR has been proven to be an interesting application to venture into (Scavarelli et al., 2020). Some think that practical in the laboratory is easier and faster causing this VR to be seen as less effective and require

complicated procedures (Hensen et al., 2020). Furthermore, this VR reduces the physical interaction of the students with the experimental materials. There are also those who express a different opinion where VR is able to help students analyze learning data better (Astuti et al., 2020) and improve student excellence in academics (Kolil et al., 2020; Su & Cheng, 2019). Figure 2 shows the example of how the students can actually analyze and observe the data in 3D model through immersive visualization. Through VR, students can focus more deeply on the practical process than playing with tools or practical materials. To solve this, it is seen that the combination between VR and practical finds the right way where the students benefit from both assessments. This is able to nurture and produce knowledgeable students in the scientific field involving genuine and real thinking (Hodges et al., 2018). This method is called Blended Reality Environment (BRE) where this method improves student performance in learning (Ryoo et al., 2018).

Another issue in the practical experiment is the students' confidence in conducting the experiment where they are hesitant to use tools and chemicals since they are the beginners to that experiment and fear the risk of accidents (Dalgarno et al., 2009). Many articles discuss the effect of preliminary planning in experiments on student performance, especially in online learning. Chaytor et al. (2017) stated that students are more prepared and confident to conduct experiments when they do preliminary preparation. This shows that students will have a better understanding of the direction of the experiment.



Figure 2: Snapshot of VR in chemistry laboratory where participant was visualizing the 3D molecular structure along with the data analysis. Picture was obtained from Nanome, Inc. Nanome: Creating Powerful, Collaborative, and Scientific VR Tools. San Diego, CA, (Nanome, 2022).

In VR practice, preliminary preparation in practical experiments can be done because it does not require a laboratory reservation and does not use excessive chemicals. This is evidence that early preparation in practice through VR can improve performance and create good experiences in student experimental practice (Chaytor et al., 2017; Kapici et al., 2020; Makransky et al., 2020; Sarmouk et al., 2019).

There are several modules applied in the initial practical preparation including the introduction of basic theory, process examples through visual cues and videos followed by simulation manuals and comprehension tests. All these modules will be open to students to be implemented for a period of two weeks and able to provide sufficient time before starting their classes, whereas the control group's pupils had access to the "conventional script and underlying theory. This strategy was carried out

by Sarmouk et al. (2019) on second-year students to assess effectiveness and impact on academic performance. Using a variety of metrics, the researchers assessed the online learning resource's performance. They employed the online tracking metrics to measure student involvement. Evaluation is made through the number of student errors that can be calculated by the laboratory assistant throughout the practical period of the experiment. Students responded to an online survey to gauge the online resource's usefulness. Based on the results of the survey, the students reported feeling more at ease overall throughout the session. In conclusion, the results of this study demonstrated that the students' laboratory experiences were improved by the online preparation with a variety of learning activities, which increased their readiness, engagement, confidence, efficiency, and performance.

When immersive VR laboratory simulations were employed in science classes, Makransky et al. (2020) discovered that students' engagement and self-efficacy rose. Comparing virtual preparations to hands-on preparations, other research discovered that there were no significant differences (Dalgarno et al., 2009; Dalgarno et al., 2012; Kapici et al., 2020). Similar findings were made by (Kapici et al., 2020), who discovered that students who participated in VR learning saw greater gains on attitude questionnaires (including self-concept) from the initial to the final than those who participated in the hands-on lessons. The final outcome showed that through the three approaches that are virtual, hands-on or combined, the three groups of students showed the same effect in terms of independence and self-confidence. The results of the questionnaire and interviews further demonstrated the virtual lesson's value, and the students indicated that they would advocate for its continued usage. However, several students claimed that unfamiliarity was not the primary cause of their fears, hence the virtual lab had little impact on their learning experience. Students realized that they are not capable to blend the chemical theory and mathematical algorithm in classroom lecture causing them to be in anxiety. The uses and impacts of VR towards education sector that affect the students' performance is summarized in the Table 1.

Table 1. Summary of recent studies on the uses and impacts of VR towards social and education sector.

Authors (Year)	Purpose	Findings
Pastel et al. (2022)	To study the effect of body visualization in VR towards body movement among different age groups.	With the use of VR, all the task demands could be completed especially for the older aged people. Implementation of VR seemed to increase the motivation and enjoyment of the participants as they found this medium was interesting to use.
Dunnagan et al. (2020)	To introduce the VR in chemistry lab and using it for the structure elucidation from infrared spectrum.	The test was conducted between two group students (one with VR aid and the other one with common experimental lab). No significant differences were observed between those two groups in terms of learning outcomes. However, students showed a great satisfaction in study using VR and it was useful to help the students

Authors (Year)	Purpose	Findings
Scavarelli et al. (2020)	To explore the use of VR and Augmented Reality (AR) in education mediums such as classrooms and museums.	who having difficulties (e.g., health care, pregnancy, self-safety) to attend the lab.
Hensen et al. (2020)	To determine the differences between actual and virtual learning environment in chemistry lab.	The authors suggested that VR/AR educational platform should be included as primary concern and also, the exploration between virtual and physical realities have to be considered for better guidance in VR/AR learning. Different grade in students' learning objectives were observed, where it was coming from the experimental procedures, not from the learning environment. Some students might found that VR was difficult to conduct in certain experiment but more efficient and less time consuming in the others. Data also showed that majority of the students achieved medium and high affective outcomes meanwhile, at about 4% to 17% of students showed low range of expected outcomes.
Astuti et al. (2020)	To study the effect of 3D visualization on students' critical thinking skills and scientific attitude in chemistry.	From the testing, 3D visualization model showed the improvement in the students' critical thinking and enhance their scientific attitude in chemistry. The proposed 3D model was classified as the excellent quality learning category.
Kolil et al. (2020)	To study the impact of virtual learning towards students' self-efficacy in experiment lab.	Virtual learning medium increased the self-efficacy among students from 88% up to 233% and polished their understanding to be better.
Qin et al. (2020)	To conduct the quantitative and qualitative analysis of VR usage in chemistry subject.	VR study should be explored and extended widely especially to promote the distance learning during COVID-19 pandemic. Final outcomes showed that through VR, students were able to interact and connect the actual environment with the theory and also the demonstrator. This actually improved the learning experience and strengthen their understanding in the syllabus. The authors were committed to continuously experimenting the use

Authors (Year)	Purpose	Findings
Sarmouk et al. (2019)	To improve the students' preparedness and performances in laboratory session through development of pre-laboratory online medium.	of VR in the classroom and more inputs will be revealed.
Chaytor et al. (2017)	To study the use of virtual pre-laboratory activities for student improvement in organic chemistry subject.	Students were reported to be interested in pre-laboratory session and found it as significant input for learning. Students were also be more confidence in conducting the experimental practice, making them to complete the session much faster than the provided time. Less error and more precision analysis was observed in students performances as the result of the pre-laboratory learning. Implementation of pre-laboratory virtual learning such as videos have increased the students understanding about the concept and practical of the experiment. Students also reported to be more prepared about the incoming experiment session and able to relate the concept and theory of the intended activities.

It has been proven that computational and simulation techniques play an important role in the world of research, especially in the field of chemistry. The atomic information obtained from this approach will be the baseline for the prediction, and modeling of various materials at different levels. Although it could be challenging to learn how to use a new simulation package from scratch, students can choose a platform that suits their interests and background thanks to the high adaptability of many software packages (whether open source or academic licenced). Interested readers can discover a number of great tutorials on related subjects (Patel et al., 2022). There are several mediums for students to access to learn MD dynamic simulation easily and quickly, for example the Chemistry at Harvard Macromolecular Mechanics interface and graphics (CHARMMing) (Jo et al., 2008). It is online access that includes Langevin and MD. Among other applications that students can explore and try are SOCOT and ChemDraw. Both of these applications are very useful for students in the field of organic chemistry where they are able to see and observe the physical characteristics, the reaction process that occurs between two reactants and the resulting products. These activities are well received by students who find computational and simulation interesting, and are committed to delving deeper into the field, but some others find it more challenging due to the learning curve of some of these complex programs.

Since each programme would offer a distinct benefit for experimental observation and simulation, we think this can be remedied by finding a better appropriate piece of software. Students can try various other interesting applications through continuous training. This can help students acquire more knowledge and skills to apply in life so that every problem can be solved. Recent studies showed the

effectiveness of Nanome through VR aids in helping and elevating the student performances in learning. Scientific study done by Qin et al. (2020) showed the impressive result on how the Nanome implementation helped the student performance where the data proved that student's performance elevated and sitting in the 4.0 or higher on 5.0 scale based on total students' evaluation as shown in Figure 3. Based on the graph, it showed that students' performances were increased in all three aspect (self-efficacy, self-assessment, and self-comfort) that obtained from self-response survey. Since 5.0 was the highest scale in the survey, it proved that most of the students were strongly agreed that VR can boost the students' performance after they have experienced the use of VR in the classroom. It was concluded that VR helped the students to visualize structure even better and improve their learning understanding (Qin et al., 2020).

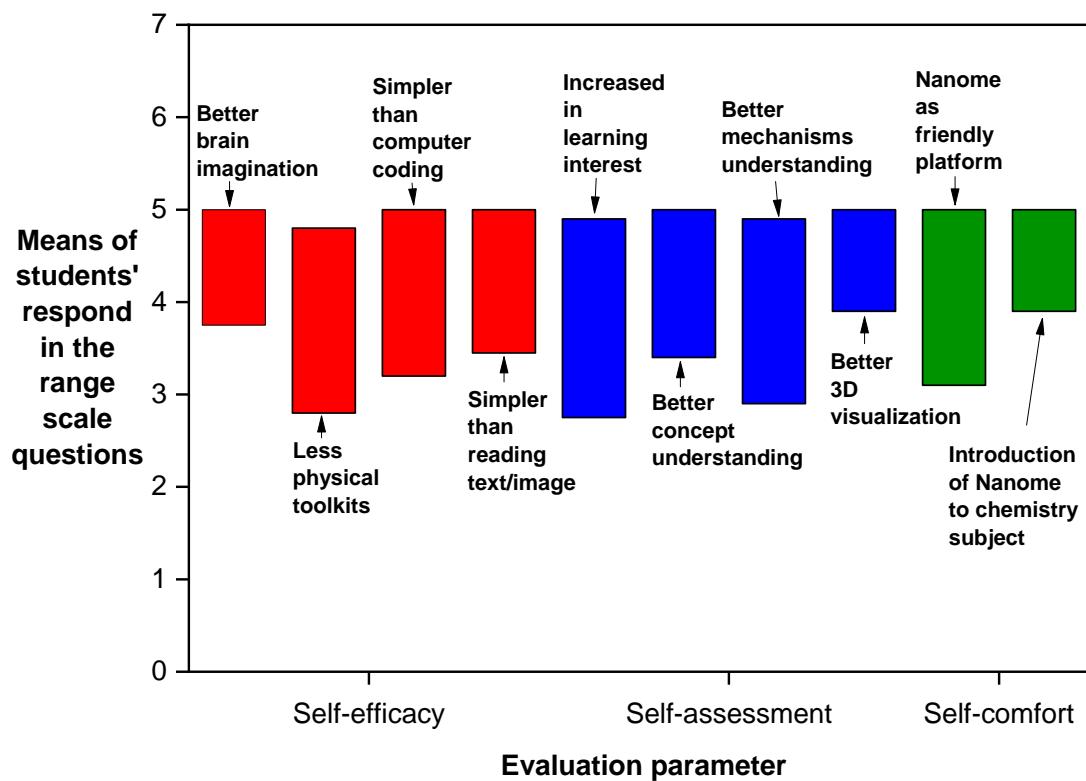


Figure 3: Evaluation of students' performances after using VR in the classroom. The evaluation was measured based on three parameter: self-efficacy, self-assessment and self-comfort through survey in range scale question. The graph is replotted based on the data obtained from Qin et al. (2020).

CONCLUSION

The use of virtual chemistry labs in pedagogical innovations for chemistry instruction has a number of benefits. Students can use the advantages of VR generally to naturally "grasp" molecules using hand controllers, as opposed to creating models using toolkits. In the end, the VR practice in learning will result in good positive impact towards students capability, versatility and adaptation towards chemical mechanism and dynamic properties of the molecules. In contrast to a computer lab, students can observe molecules without being constrained to a 2D screen or having to learn programming languages. Finally, the VR lab stimulates curiosity, and many students discovered that learning chemistry was more concrete and enjoyable.

RECOMMENDATION

For future research in VR study, the scope will be widely open to other fields and sections such as sports, cultures, music, and arts that can be implemented for different ages and levels (school, community and organization).

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