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Technology Report

Introducing Atomic Structure to First-Year Undergraduate Chemistry Students with an Immersive Virtual Reality Experience

Nadezhda Maksimenko, Anzhelika Okolzina, Anna Vlasova, Chantal Tracey, and Mikhail Kurushkin*

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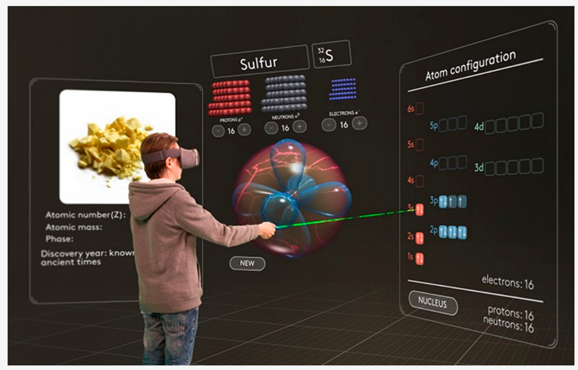
ABSTRACT: The present technology report is aimed at demonstrating how the implementation of VR chemistry simulations of atomic structure enhances learning among students. MEL Chemistry VR lessons were incorporated into the classroom for 43 first-year undergraduate ITMO University students. The visualization techniques provided the learners with two important opportunities: (1) connecting the macroscopic and tangible component of chemistry with the submicroscopic component (the real world and the world of molecules) and (2) connecting the submicroscopic component of chemistry with the representational one (atomic structure and orbital diagrams). The results show that implementation of the VR experience into the atomic structure laboratory enhances the learning experience of the students.



KEYWORDS: *First-Year Undergraduate/General, Physical Chemistry, Computer-Based Learning, Atomic Properties/Structure, Periodicity/Periodic Table*

OPPORTUNITIES FOR VISUALIZATION IN CHEMISTRY EDUCATION

Chemistry as a science incorporates many abstract concepts and terms, making it challenging to understand. Some sciences are more challenging to understand than others because of the number of abstract concepts and terms. Chemical compounds exist in reality, but we cannot see their molecular structure with our bare eyes. The deeper we go into ordinary things, the more problems we meet in visualization of small particles. This is a common problem for chemistry, physics, and biology. Ball-and-stick models[1] and animations[2,3] have been able to solve it to some extent. However, recent technologies provide a wider range of opportunities for visualization.

Augmented reality (AR) and virtual reality (VR) technologies (AR adds digital elements to a live view, often by using a camera on a gadget,[4] while VR implies a complete immersion experience[5]) allow improvement of science courses at school or university,[6,7] and some of them even include a laboratory component.[8−10] When it comes to dangerous, toxic, radioactive, and carcinogenic substances, simulation technologies are safer and less expensive[8,11−13] than classical laboratories. The ability to manage dangerous substances safely in the laboratory is an important component in laboratory education that definitely cannot be substituted with VR. However, the question of the cost of some reagents of this kind as well as the question of the safety of their storage in the laboratory can be solved by using VR technologies. Moreover, it does not require special places for work or equipment storage, and as online education becomes increasingly popular, 3D VR provides a unique opportunity not to skip such an essential part of the chemistry education as laboratory practice.

Most of the things that are introduced in a chemistry laboratory are macroscopic by nature. Nevertheless, chemistry cannot be fully understood without going to the submicroscopic level.[14] It is considered that chemistry consists of three components, which can be considered as corners of a triangle:[14,15] (i) the macroscopic and tangible (what can be seen, touched, and/or smelled); (ii) the submicroscopic (atoms, molecules, ions, and structures); and (iii) the representational (symbols, formulas, equations, molarity, etc.).

There are several papers on immersive VR in chemistry education[16−25] that are focused on organic and biomolecules in order to simulate what types of rotations and reactions are possible with them. Various approaches for the implementation of operating molecules using AR have been reported.[4,26−28] Such kinds of simulations that allow students to interact with molecules in real time, notably immersive molecular dynamics in virtual reality, have become technically available only recently.[17,18,22,25]

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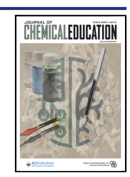

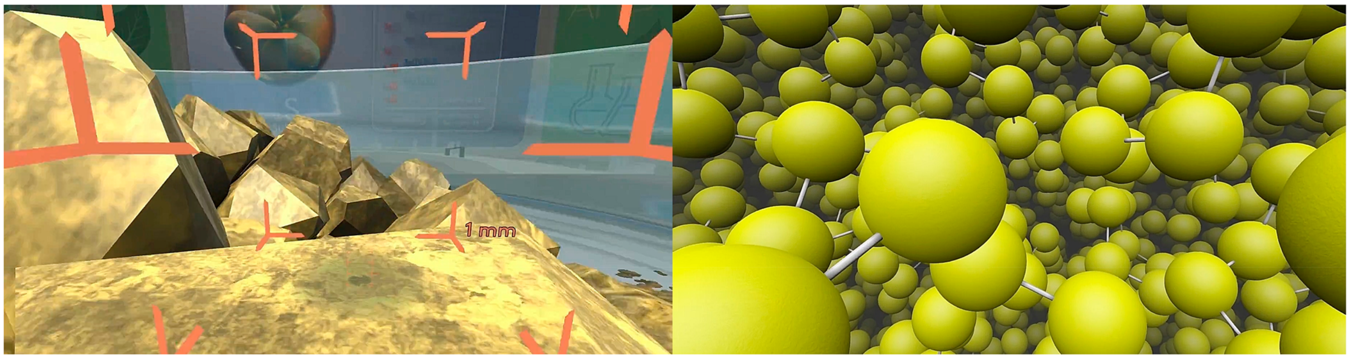

Figure 1. Screenshots from the VR experience: (left) the start and (right) the end of zooming into the crystal structure of sulfur.

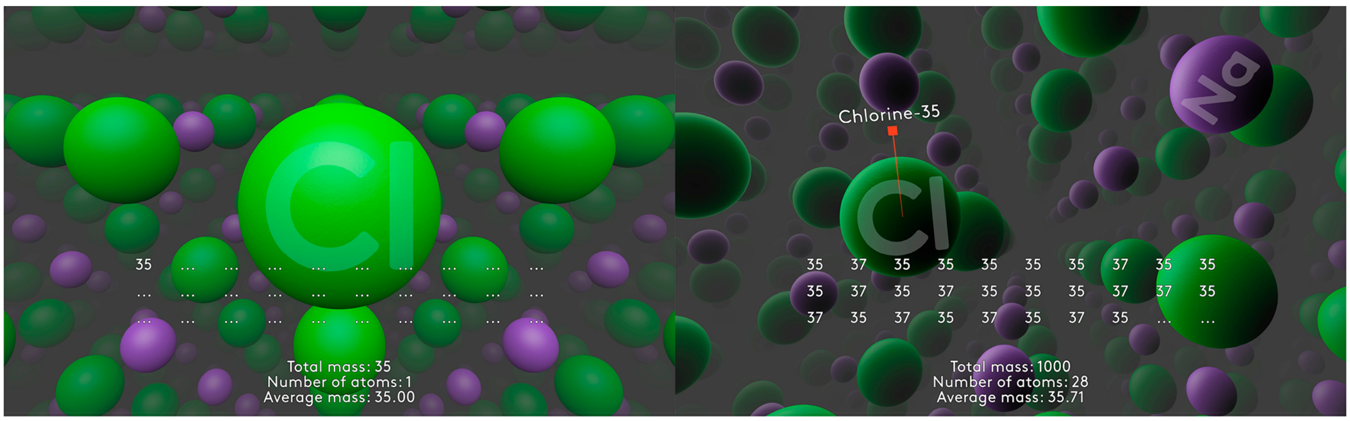

Figure 2. Screenshots from the VR experience: (left) the start and (right) nearly the end of picking chlorine ions with different mass numbers.

However, there are very few articles dedicated to the introduction of immersive virtual reality in chemical education for visualization of objects that are smaller than molecules, i.e., atoms and their structure.[5,29] In the present study, we incorporated VR chemistry simulations of atomic structure into the classroom for undergraduate students in order to describe its implementation and show how it enhances learning. Despite the fact that various resources offer 3D lessons on various chemistry topics aligned with most of the K12 ("K through 12", from kindergarten to 12th grade) chemistry curriculum, the MEL Chemistry VR Lessons platform[30] (an educational platform that offers immersive AR and VR lessons) stands out because of the unique realistic visualizations of atomic nucleus structure and atomic orbitals that are not offered elsewhere, which motivated its choice for the present technology report.

■ MEL CHEMISTRY VR LESSONS

MEL Chemistry VR includes free lessons that allow learners to get a completely immersive experience with the ability to interact with the virtual reality objects. The software supports most mobile VR platforms, including Google Cardboard, Oculus GO, GearVR, and Pico VR, and can be run in non-VR mode on tablets. Each lesson is 3–7 min long and can be integrated into the classic lesson flow, making the subject more visual and comprehensive. Teachers control the lesson flow using the special VR teacher mode on a tablet device. In this mode, all student devices on the same Wi-Fi network are instantly connected to the teacher's device, allowing the teacher to start and pause the lesson as well as to control the progress of each student.

Each lesson starts in a lab and then zooms in to the molecular level, including the lesson dedicated to orbital names (Figure 1). These visualizations are based on the laws of physics, and one of the features of the zooming is that as learners "shrink up" to a billion times, they are able to observe realistic models of the atomic nuclei, including the protons and neutrons that constitute them. With the help of these tools, students will either visualize crystal structures according to ball-and-stick models (Figures 1 and 2) or artistic renditions of Bohr's model (Figure 3).

Such use of VR technology helps overcome one of the main difficulties in chemistry education: connecting the macroscopic and microscopic worlds in an overall concept and seeing how they are linked. Many of the lessons offer interactive experiences on the molecular level. Interaction with atoms that would otherwise be impossible can be conducted, such as building atoms and simulating their properties with input results, etc. An important feature of these manipulations is that the students can interact with virtual atoms, explore and change their makeup, rotate them 360°, and witness the corresponding orbital diagrams with electron distribution at the same time. During the atomic mass lesson, students have a chance to become as small as an ion and "fly" through crystal structures (Figure 2).

Hence, the VR experience supports students in connecting the real world of chemical substances and the submicroscopic world as well as connecting the latter with the representational language of chemistry.

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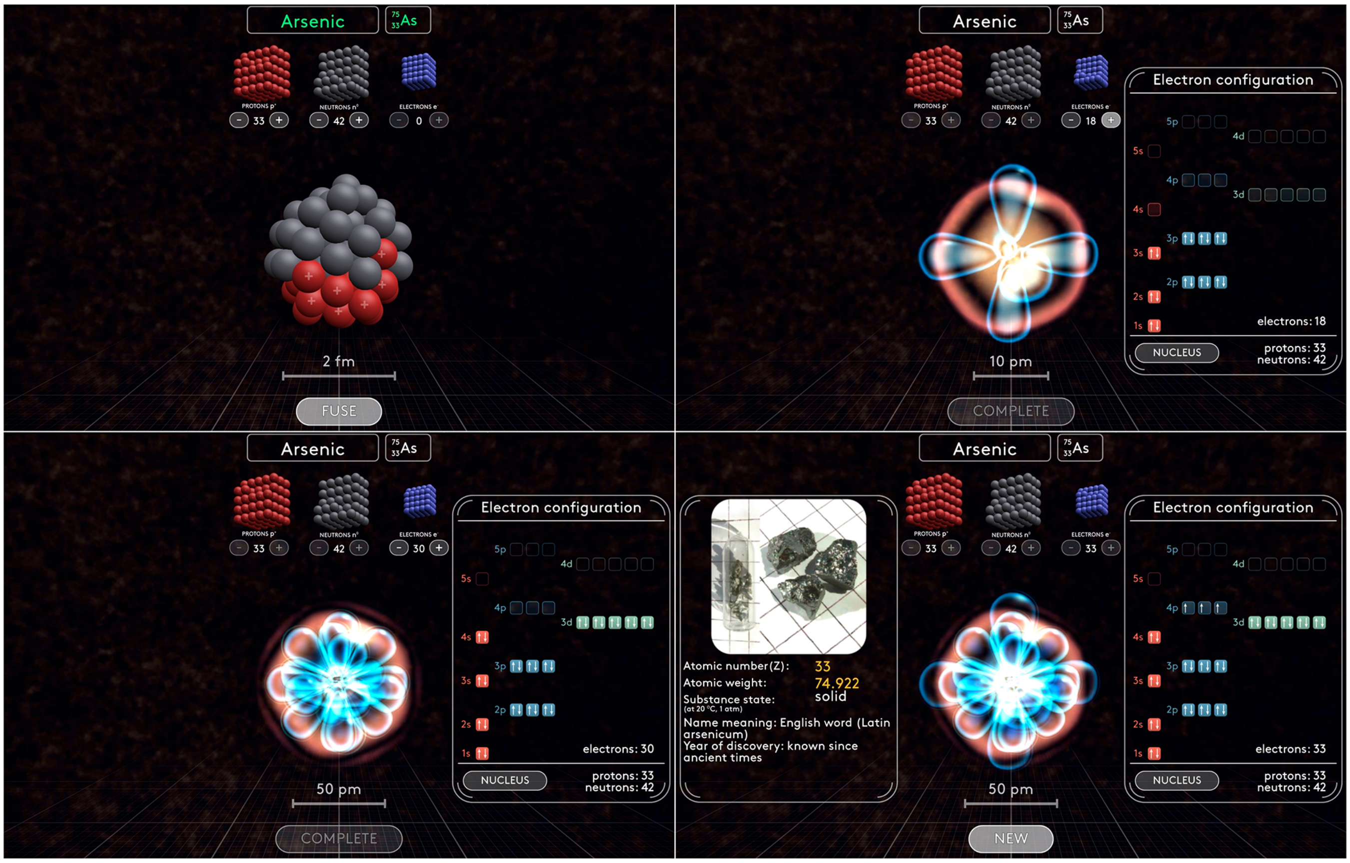

Figure 3. Screenshots from the VR experience: (top left) picking the suitable number of protons and neutrons for an arsenic-75 nucleus; (top right) completing the electron configuration up to 3p; (bottom left) completing the electron configuration up to 3d; (bottom right) finalizing an atom of arsenic-75.

■ IMPLEMENTATION OF MEL CHEMISTRY VR LESSONS IN THE CLASSROOM

The main goal of this work was to show that after virtual lessons students will have a better understanding of the structure of the atom because this concept is often confusing to students and difficult for the teacher to explain. Despite this fact, grasping the nature of atomic structure is a basic requirement for the subsequent identification and understanding of laws in chemistry. The MEL Chemistry VR laboratory called “Make your atom” is a practical activity that provides the students with the opportunity to build any atom of any known stable isotope of elements through hydrogen to bismuth (except technetium and promethium). The students start by choosing a combination of protons: as each proton is added, the element with the corresponding atomic number appears at the top of the screen. Next, when the number of protons is selected, neutrons are added: if the user adds the wrong number of neutrons in the nucleus, the constructor does not allow adding electrons. When the nucleus of an atom is assembled correctly, the user is able to add the electrons one by one, and they are displayed on the electron diagram (on the right side of the screen), and all of the atomic orbitals are highlighted with a virtual laser. When the entire atom is assembled correctly, the user is able to rotate the resulting atom 360°, and information about the chemical element is displayed on the left side of the screen (Figure 3).

This lesson was implemented into a chemistry classroom with 43 first-year undergraduate students studying chemistry at ITMO University in September 2020. The design of the experiment was quite simple: before the class, students were asked to write electronic configurations and orbital diagrams and to draw the electron clouds for atoms of four elements from the periodic table as a pretest (the PDF version of the test is provided in the Supporting Information). After completing this task, they were given the opportunity to make their atoms in the immersive virtual reality and see the numbers of protons, neutrons, electrons, their mutual locations, artistically rendered polar plots of the real angular terms of the atomic wave functions, and the orbital diagram of any atom they assembled. Eight Oculus Go headsets were implemented during this classroom; this choice of headset is explained by its convenience and ease of use and the fact that its use does not occupy too much space. Then they wrote the post-test with the same task (the PDF version of the test answer key is provided in the Supporting Information) but different elements. Each student took part in the pretest, the VR experience, and the post-test over the course of 2 academic hours. The maximum possible test score was 16 points (4 points per element).

■ EVALUATION

The results of the experiment show that 27 students managed to get a higher score on the post-test than in the pretest, while the score decreased for four students and 12 students had the same score on the pretest and the post-test. The pretest showed that students had trouble in understanding what orbitals look like and how the electrons are distributed the most before the VR experience. Besides, the best score for the

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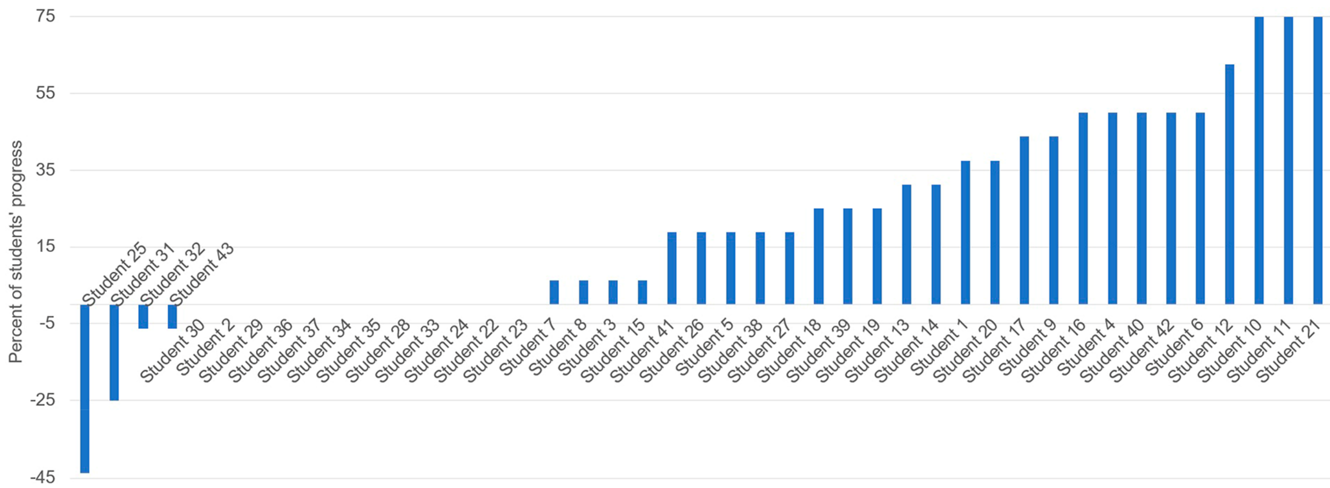

Figure 4. Percent of students' progress based on comparison of pretest and post-test scores (from lowest progress to highest).

post-test was 15 points. The average score on pretest was 6.000 ± 2.930, and on the post-test it was 9.260 ± 2.901. It was estimated that the average percent of progress was 20.3% (Figure 4).

The progress results in going from the pretest to the post-test can be evaluated by comparing the results using the two-sample Student's t test in order to test the hypothesis of a difference between two dependent samples—in our case, to understand whether the laboratory lesson was the reason for improvement of the test results, while the alternative hypothesis was that the use of MEL Chemistry laboratory had no impact on the students' results. To calculate the empirical value of t in the situation of testing the hypothesis of differences between two dependent samples (in our case, two samples of the same test with a time interval), the following formula is used:

$$t = \frac{M_{\mathrm{d}}}{s_{\mathrm{d}}/\sqrt{n}}$$

where M_{d} is the average difference of the values, s_{d} is the standard deviation of the differences, and n is the number of observations.

The calculated t value is 5, which it is larger than the tabular critical value (which is 2.7 for $\alpha = 0.01$ (one tail)), which means that for this level of significance the differences between our samples are considered statistically significant. Hence, the implementation of this technology to chemistry classes is able to help the understanding of the atomic structure through realistic visualizations that students can see in computer models, such as MEL Chemistry VR lessons.

CONCLUSION

The present technology report indicates that the implementation of an immersive VR experience involving atomic structure, periodicity, and periodic table lessons can considerably influence learning outcomes of students. Therefore, the VR experience can be seen as a useful tool for enhancing students' understanding of chemical concepts, and it is essential for a better perception of abstract notions that cannot be otherwise visualized in full detail. Interaction with particles, atomic nuclei, atomic orbitals, and atoms can facilitate the learning process of difficult chemistry concepts by visualizing these objects in the immersive virtual reality.

An important advantage of the VR lessons is the availability and compatibility with most mobile VR platforms, including Google Cardboard, Oculus GO, GearVR, and Pico VR. Hence, a traditional chemistry classroom can be equipped for immersive VR lessons at a relatively low price compared with more technically elaborate equipment that requires lengthy preliminary instructions, additional free space, and more expensive gear, such as HTC Vive. It is important to note that the MEL Chemistry VR lesson "Make your atom" is freely available.

In the present technology report, we are able to argue that the implementation of this technology in chemistry classes improves the understanding of atomic structure. At the same time, we believe that VR technology is a helpful tool that is intended to support a skillful chemistry educator and the students' own efforts in self-learning with the help of textbooks and other sources. The VR technology itself is not meant to and probably should not substitute for real laboratories or teachers. We hope that the findings presented in this technology report draw the attention of chemistry teachers and instructors to the possibilities offered by immersive virtual reality and support their efforts in teaching the essential topic of atomic structure.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c01441.

Pretest and post-test (PDF)

Test answer keys (PDF)

AUTHOR INFORMATION

Corresponding Author

Mikhail Kurushkin — *Chemistry Education Research and Practice Laboratory, SCAMT Institute, ITMO University, Saint Petersburg 191002, Russian Federation;* orcid.org/0000-0001-9031-8247; Email: kurushkin@scamt-itmo.ru

Authors

Nadezhda Maksimenko — *Chemistry Education Research and Practice Laboratory, SCAMT Institute, ITMO University, Saint Petersburg 191002, Russian Federation*

Anzhelika Okolzina − *Chemistry Education Research and Practice Laboratory, SCAMT Institute, ITMO University, Saint Petersburg 191002, Russian Federation*

Anna Vlasova − *Chemistry Education Research and Practice Laboratory, SCAMT Institute, ITMO University, Saint Petersburg 191002, Russian Federation*

Chantal Tracey − *Chemistry Education Research and Practice Laboratory, SCAMT Institute, ITMO University, Saint Petersburg 191002, Russian Federation*

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.0c01441

Notes

The authors declare no competing financial interest.

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