
Developing a Virtual Reality Approach Toward a Better Understanding of Coordination Chemistry and Molecular Orbitals

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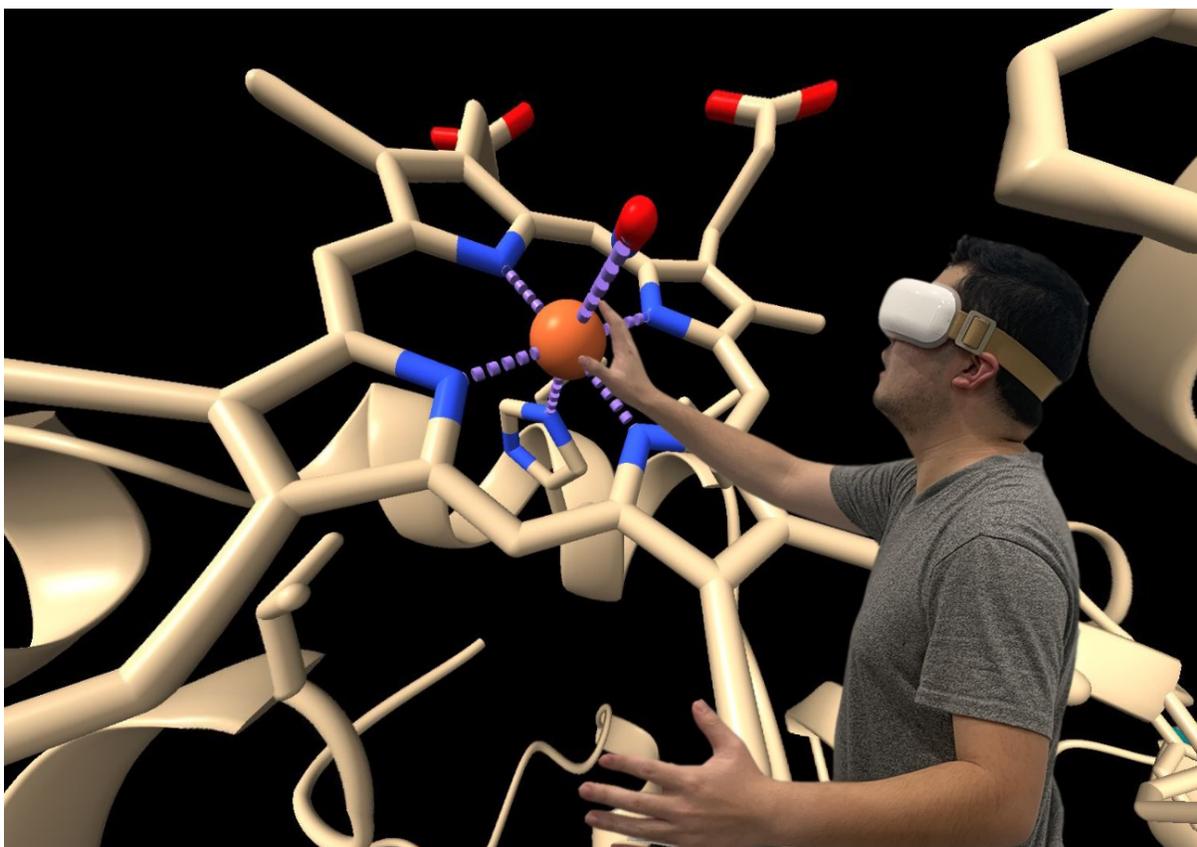
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ABSTRACT

A virtual reality (VR) session was introduced to an advanced inorganic chemistry class, a class available to junior and senior undergraduate students at the University of California, Los Angeles. The
10 VR session helped the students to learn complicated aspects of metal coordination chemistry and molecular orbitals via an immersive three-dimensional experience.

GRAPHICAL ABSTRACT



KEYWORDS

15 Upper-Division Undergraduate; Inorganic Chemistry; Computer-Based Learning; Coordination
Compounds; MO Theory

Coordination compounds and molecular orbitals are two important concepts in the inorganic
chemistry education of undergraduate students.¹⁻⁴ Relaying these concepts is difficult because the
20 molecular scale is far removed from that of everyday objects. Additionally, as the structures become
increasingly complicated, it becomes difficult to engage the students. For example, when discussing
heme, simplified structures are commonly used (Figure 1). However, such models do not help the
student to understand coordination via a tetradentate ligand, nor how the heme is part of the
hemoglobin structure. This problem is exacerbated when teaching molecular orbitals, as there are not
25 too many toolkits available.

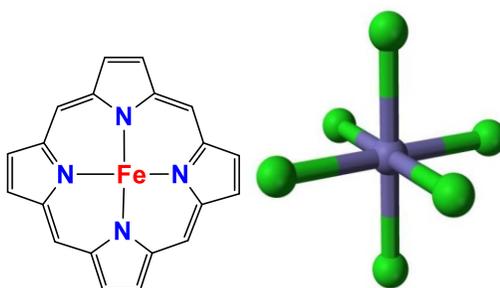


Figure 1. Simplified representations of iron-heme complex (left) and an octahedral coordination compound (right).

Virtual reality (VR) is a powerful emerging technology that allows the user to be fully immersed
30 within a three-dimensional experience. Virtual reality is currently being used for a variety of
educational purposes, including remote classroom settings. Examples of science education
applications include: MEL Science,⁵ Nanome,⁶ UnityMol,⁷⁻⁹ EduChem,¹⁰ VR-Engage,¹¹ a calorimetric
titration app,¹² and ChimeraX.¹³ Combining the VR technology and a chemistry class could become a
new and fascinating teaching method. Fung et al.¹⁴ reported conducting a VR field trip for an
35 environmental chemistry class. A 360° video was made during the actual field trip and transferred into
a VR compatible video file, which was later viewed by students in the classroom. This approach saved
time and resources for the class. However, it lacked interactions, meaning that the students could see
everything with the 360° view but could not get close to, manipulate, or interact with objects such as

flipping or moving something around. If a higher level of interaction is to be achieved, a model should
40 be built in VR instead of using a video. Ferrell et al.¹⁵ reported the use of VR in a laboratory chemistry
class, where students gained a straightforward understanding on how the size of organic molecules
affected their boiling points. Bennie et al.¹⁶ reported the use of VR in a computational chemistry class,
where the students were instructed to construct enzyme structures computationally and then perform
real-time interactive molecular dynamics simulations in VR. The last two publications showed the
45 great potential of VR teaching in organic chemistry and biochemistry. Herein, we report the first
example of using interactive VR for an advanced inorganic chemistry class, giving students the chance
to observe and manipulate objects in depth in a VR session.

VIRTUAL REALITY SETUP AND MODEL FILES

An HTC Vive virtual reality system was used as the VR interface and was connected to a standard
50 gaming PC (CPU: Intel i7-6700K, GPU: NVIDIA GTX980). Two tracking cameras were used to measure
precisely the movement of the VR headset, and two controllers to allow for interactions with VR
objects. UnityMol and ChimeraX were employed as the data visualization software. The VR compatible
files were previously generated computationally. The structure of hemoglobin was downloaded from a
published paper,¹⁷ and the crystal structure as well as computational studies for (salfen)Zr(OⁱPr)₂
55 (salfen = N,N'-bis(2,4-di-*tert*-butylphenoxy)-1,1'-ferrocenediimine) were previously reported by our
group.¹⁸ The molecular orbital the students observed was the lowest unoccupied molecular orbital of
(salfen)Zr(OⁱPr)₂.

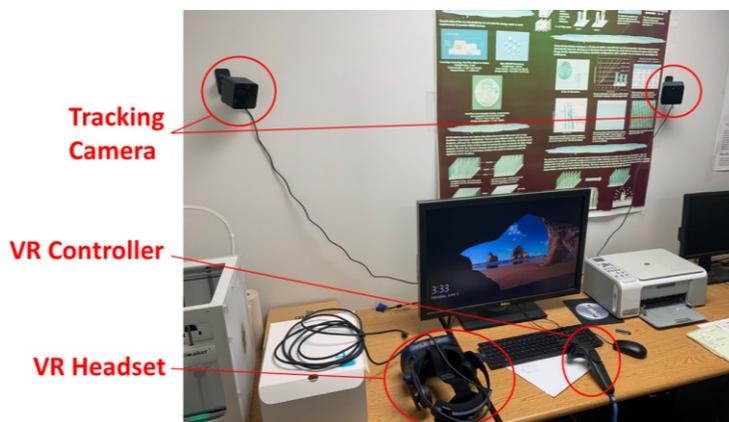


Figure 2 VR setup used during student sessions.

In order to provide a meaningful VR viewing/learning experience, a one-on-one teaching method was adopted, with each student engaged in a 30 minute session. Overall, 32 out of 71 students signed up for the VR session voluntarily, and no bonus points were awarded for participation. As such, the rest of the students acted as a non-controlled comparison group.



Figure 3 TA helping students getting used to the VR setup.

The VR session objectives were:

- (1) allow the students to become familiar with VR tools, starting with the hemoglobin structure;
- 70 (2) allow the students to observe the coordination environment of iron and understand the coordination site;
- (3) show the students a relatively complicated metal complex;
- (4) teach the students to identify the atomic orbital components of a specific molecular orbital.

The students were first shown the structure of hemoglobin (Figure 4a).¹⁷ The starting viewpoint was
75 at the center of the hemoglobin structure, and the student could manipulate the image (Figure 4b). It took two to three minutes before students became fully used to the VR “world” and performed translations and rotations of the molecule with the VR controllers. The students were asked to find all the four heme groups inside hemoglobin. Then, the students chose one heme group, moved it closer to them, and they were asked to find all the donor atoms bound to the iron center. Most students agreed
80 that interactions in VR helped them to understand the coordination environment of heme, how the

other heme units are spatially resolved, and the impact of the protein fold on the localization of heme groups in hemoglobin, compared to merely viewing 3D images on a 2D screen.

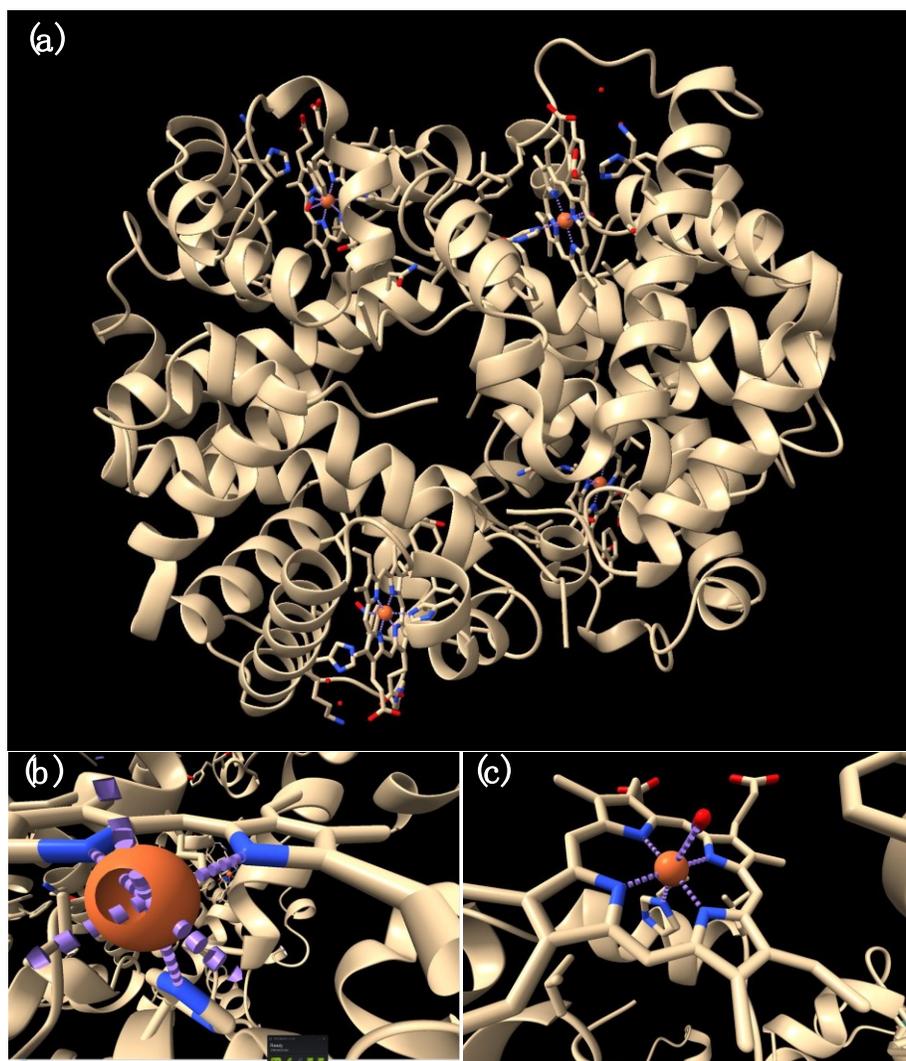


Figure 4 (a) The overall hemoglobin structure (PDBID 3WCU) in VR, (b) a zoom-in inside the protein, next to a heme group, (c) a close look at the heme group.

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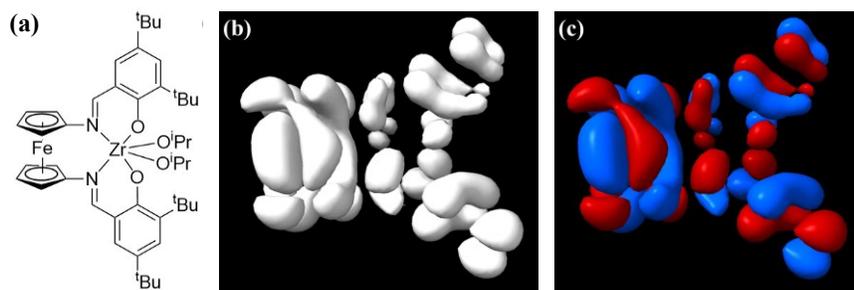


Figure 5 (a) Drawing of (salphen)Zr(OiPr)₂; (b) the original all white lowest unoccupied molecular orbital; (c) the molecular orbital phases distinctly colored.

Table 1. Results of the anonymous survey after the VR session; 32 students (100% of participating students) took the survey.

Entry	Question	Average score
1	Have you ever used a VR set (for education/gaming or anything)?	Yes 37%
	Yes or No	No 63%
2	What do you think of your TA's instruction?	8.8/9
	0 = bad; 9 = very informative	
3	What do you think of this VR facility?	8.4/9
	0 = old school; 9 = very modern and advanced	
4	How do you physically feel about VR viewing?	8.3/9
	0 = physically uncomfortable, dizzy; 9 = I'm good	
5	Do you think a 30 minute time slot is enough?	5.2/9
	0 = enough, I feel bored already; 5 = right amount, impeccable; 9 = no, I need more time	
6	Do you think this VR experience helped you with the class?	7.9/9
	0 = no, just a waste of time; 9 = very helpful, it helps me to understand MOs better	
7	After this VR experience, do you want other science classes to adopt VR?	8.6/9
	0 = no, please limit it to this class only; 9 = I want to use VR in other classes as much as possible	
8	Overall, how do you rate this VR experience?	8.6/9
	0 = horrible; 9 = wonderful	

The students were then shown the 3D model of the lowest unoccupied molecular orbital of (salfen)Zr(OⁱPr)₂ (Figure 5). Students were first asked to paint colors on the original all-white orbital (Figure 5b) to give a color-coded orbital (Figure 5c), in order to obtain an impression of the different phases of the molecular orbital. Then, the chemical structure of the compound was given in order to identify the orbital contributions of the ferrocene unit, phenoxide rings, and zirconium center. Finally, the students were asked, for each orbital segment, if the drawing had a reflection plane or an inversion center. The orbital coloring task is a bit challenging but doable. The students need to (a) identify the type of atomic orbitals contributing to a specific molecular orbital, and (b) figure out inversion or reflection symmetry based on the specific phases of atomic orbitals. Such knowledge was mentioned extensively in the lectures, and students were given on-paper practice to solidify those concepts.

Each of the four tasks took students about three to five minutes, and most of them agreed that the VR experience helped them to understand the concept of molecular orbitals better than just using the images provided in class.

ANALYSIS OF LEARNING RESULTS

At the end of the session, each student took an anonymous survey about their experience with VR (Table 1). According to the results, for most of the students, this was their first VR experience (entry 1). Despite not being exposed to VR before, they all learned how to control the visual angle in VR quickly, and how to manipulate the molecules with the controllers. Considering there were reports of people having visually induced motion sickness (commonly known as 3D sickness),^{19,20} we specifically asked the students about their physical experience; no problems with VR viewing were registered (entry 4). In addition, the students thought that a 30 minutes time slot is the right amount of time to enhance their learning experience (entry 5), and it did help them understand the concepts of molecular orbitals and coordination structures better (entry 6) than just using the class material. Overall, the students gave a positive feedback about their VR experience.

Table 2. Score analysis of the students who took the VR session and those who did not.

Category of students	Overall average scores ^a	Average score increment from 2 nd midterm to final exam ^b
Enrolled in the VR session (32)	83.1	18.6
Not enrolled in the VR session (39)	76.8	17.2
The whole class (71)	79.6	17.8

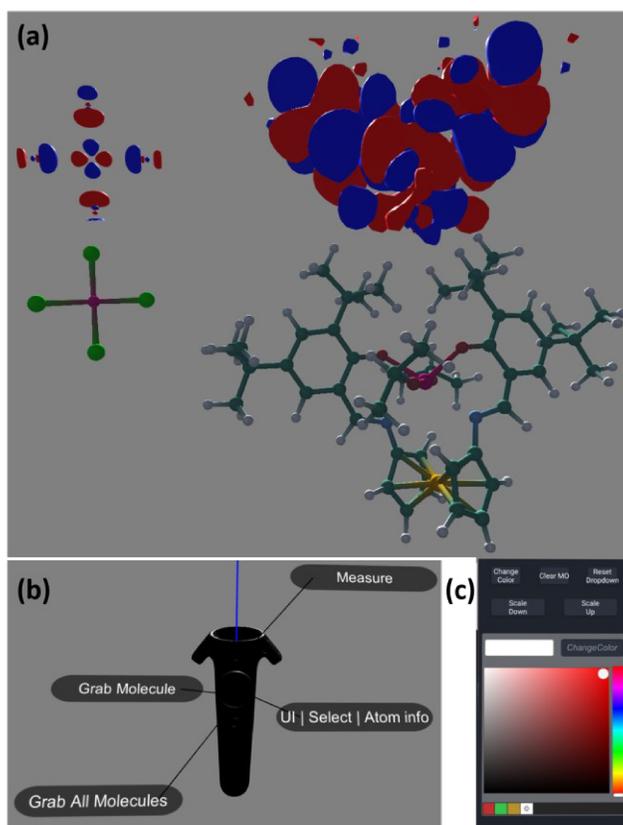
^a Scores are out of 100. ^b Represents the final exam score minus the second midterm score since the VR session took place after the second midterm and before the final exam; scores are out of 100.

We also performed a score analysis at the end of the teaching quarter (Table 2). Since it was not mandatory for the students to sign up for the VR session, a non-controlled comparison group for learning was formed between the students who took the VR session and those who did not. We found that the students who took the VR session had an overall average score higher than the students who did not, indicating that students might be benefiting from using VR. Furthermore, since the VR

125 session took place after the second midterm exam and before the final exam, we also analyzed the
score increment from the second midterm to the final exam. The results show that the students who
enrolled in the VR session had a higher average score increment than those who did not. However, it is
possible that the students who were willing to enroll in the VR session may be more motivated than
those who did not, meaning they would excel in the class regardless of the VR session.

130 **FURTHER IMPROVEMENT OF SOFTWARE AFTER TEACHING**

Although the students found the VR session useful, we noticed that there was some room for
improvement. For example, students frequently took off the VR headset to read their handouts, then
put on the headset to continue the virtual interaction with the molecular orbitals; such a switch is not
convenient. In addition, students needed to take off the headset to add color to the molecular orbitals
135 on the computer monitor. We decided that the experience could be improved if students could perform
all those tasks with their VR headset on.



140 Figure 6 (a) UnityMol allows loading multiple objects simultaneously, thus a direct comparison of ball and stick models with molecular orbital data is possible. (b) An in-app view of the HTC Vive controller with labels displaying the action for each label. (c) Menu for molecular orbitals that allows users to resize and color accordingly.

Therefore, we decided to test a new software, UnityMol,⁷⁻⁹ which allows to implant a simple document (e.g., a handout) into the VR user's interface. UnityMol allows many functions to be completed within the virtual interface such as loading a new file or adding color to a specific molecular orbital, allowing a streamlined experience for the students during the VR session. In Figure 6b, a picture from the user's point of view is shown with instructions for each button directly labeled on the controller. The UnityMol software also allows users to load multiple molecular orbitals, making it easy for students to compare them. Figure 6c shows the menu that allows coloring of each phase of the molecular orbital as well as resizing the objects.

UnityMol turned out to be a great VR platform for teaching molecular orbitals, because it offers an improved immersive experience, where everything can be done without taking off the headset. However, it is worth mentioning that the ideal time for each UnityMol VR session should be at least 30 minutes, since the students need time to get accustomed to the interface. On the other hand, ChimeraX is suitable for fast VR sessions, where the teaching assistant types in the commands and students only focus on the molecular orbitals, therefore, each session can be shortened compared to a UnityMol VR session.

CONCLUSIONS

The advancement of VR technologies will allow their standard application in science education. For objects that cannot be seen in daily life, e.g., molecules, molecular orbitals, microorganism and human tissues, VR viewing is a powerful educational tool that enables the students to view from every direction, even inside the objects. Moreover, with the help of VR controllers, the students can interact with the objects in the VR mode, making the experience similar to viewing in real life.

As the first case of applying VR technology in inorganic chemistry, our advanced inorganic chemistry class provided each student with a 30-minute VR viewing session. The students went through the 3D structure of hemoglobin and the molecular orbitals of (salphen)Zr(OⁱPr)₂. The students all gave a positive feedback, making us confident that this teaching method is valuable.

Based on the student feedback and the teaching assistant's observations, we realized that it would be better to upgrade our VR software platform, therefore, we incorporated UnityMol as another teaching tool. This improvement should allow an improved experience for students.

170 ASSOCIATED CONTENT

Supporting Information

The detailed results of the post-class survey (DOCX) are available as a Supporting Information file on the ACS Publications website at DOI: 10.1021/acs.jchemed.XXXXXXX.

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