VSPER Theory, An Interactive and Immersive Learning Environment

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***Abstract*—In this work, we are exploring the role of immersive learning in regards to predicting molecular structures and orbital hybridization. Specifically, we utilize an interactive virtual learning environment to help teach the concept of the Valence Shell Electron Pair Repulsion theory. We developed an interactive and immersive simulation in which participants constructed virtual molecules. Following the simulation, we conducted the a study using the Game Experience Questionnaire to assess the level of Immersion. We also asked participants to identify shapes of similar molecules to measure their understanding of the theory as compared to a control group. The results show that our virtual learning environment experience improves comprehension of three dimensional structures in chemistry.**

***Index Terms*—Virtual Reality, Immersive Learning, Visualization, Virtual Learning Environment, Orbital Hybridization, VSPER theory, Molecular Structures, User Study**

I. Introduction

In Chemistry and Physics, the geometric properties of atomic bonds are of essential interest; The shape of molecules as well as crystal structures are governed by the laws of Valence Shell Electron Pair Repulsion (VSPER) [1]. Depending on the electron configuration of the valence band, only certain spots distributed spherical around the atom can be occupied by bonds to other atoms. This leads to certain, predictable regions where bonds can occur and consequently a distinct bounding geometry. For example, water has two hydrogen atoms bond to oxygen in a bent shape of $104.5°$ and not linear (180°), based on the electron repulsion from the involved valence-electrons: Two electron-pairs bond and the four remaining, free valence electrons from oxygen share the possible space around the atom [2]. Gillespie [3] [4] differs between weak and strong bonds. While the weak bond interaction is dealt with by the Kepert model [5] , the strong interaction generates bonds in an antipodal configuration along the sphere [6] [7] such as in a carbon dioxide.

The bond angles rely on the electron-configuration, in particular, the number of valence electrons and how many are shared in a molecule to achieve a complete valence band. The configuration is distributed evenly on a spherical surface representing the atomic shell. Two-dimensional illustrations are subject of strong abstraction and lack the ability to convey the spatial nature of the topic. The common learning materials are static two- and three dimensional images. In both cases, depth impression is absent, therefore, the illustration is often reduced to a two dimensional representation in order to not overload the visuals. Furthermore, the bond angles are not only defined by the spatial distribution of the valence electrons, but also on how much of these valence electrons are involved in the binding: Carbon has six evenly, non-antipodal spatial spots for its valence band, but if it forms two sets of double bonds with oxygen, an antipodal configuration is set. Visualizing such transition in an interactive virtual learning environment (VLE) has a strong potential to convey a basic understanding of the topic. Virtual Reality (VR) makes it possible to immerse the learner into a Virtual Learning Environment [8] [9] [10] that is enhancing, motivating and stimulating learners' understanding of certain events [11] [12]. Interactive VLE's have shown the ability to transmit physical phenomena surpassing traditional learning methods [13] [14]

Our novel Virtual Learning Environment approach utilizes virtual reality (VR) and interactivity to teach VSPER theory. In our VLE, electrons are animated, "orbiting" the atom along a path described by its wave function. Students can interact with different atoms and identify the spatial space occupied by the valence band electrons. Moreover, the user can attach different atoms until the valence band of the involved atom is complete, experiencing the transition of possible attachment points depending on the valence configuration and the amount of shared electrons per bond. The VLE is designed to teach VSPER theory through activities that help the learners establish a common sense of the possible configurations of spatial bonds and to predict a variety of different bonds.

In order to measure the effectiveness of the VLE, we conducted a user study in which one group of learners used our VLE, and the other, control group was taught using a traditional learning methods.

II. Methodology

For this study, we developed an interactive and immersive simulation which allowed participants to build simple molecules in order to enhance their competence in regards to molecule bonding configurations. We asked participants to build nine different molecules, with three particular atoms and six distinct resulting shapes.

The VLE presents a set of atoms to construct molecules and its physical model is based on Schroedinger's [15], [16] valence bond theory, VSPER describing orbits as wave functions, which is further important to understand the potential (three dimensional) occupation of binding space around an atom. Our VLE does not expand to isovalent hybridization [17] or Bent's rule [18] to explain the hyperfine deviations of the bond angle, because that would involve a different physical topic, which is outside the scope of our work. However, these deviations are minor and are not required in order to understand the principle of valence bond theory.

We tested a group of n = 69 participants and conducted our research in three steps. First, we used a pre-questionnaire to assess their demographics and to show a sample question on molecular geometry with respect to VSPER theory. Next, participants engaged with one of two lessons. A set of n = 42 volunteers used our Virtual Learning Environment, which taught participants how to predict a molecule's atomic geometry configuration. For our control group, a set of n = 27 participants instead completed a traditional learning experience. Finally, each answered a post-questionnaire to determine their gain in understanding of VSPER theory and level of immersion. Immersion was measured using two different sets of questions to determine how participants felt during and after the VR experience [19], [20].

A. Orbital Hybridization Simulation

1) Development: Our VLE immerses players by entering them in a virtual reality world. We designed our virtual world using Unity and Oculus Unity Integration. Players observed the world with an Oculus Rift HMD, allowing users to look in any direction. The world was interactive, so players completed simulation tasks using a pair of Oculus Touch controllers. Participants interacted with the virtual world by grabbing, releasing, and throwing objects, by squeezing the grip button on the Oculus Touch controller. We ran our Unity simulation on a Windows 10 Desktop with a Intel Xeon E5-1620 CPU, 32 GB of memory, and a Nvidia GeForce GTX 980 GPU.

Our research required that our VLE simulates atomic bonding behavior among model atoms. Therefore, our Unity simulation includes logic for atomic bonding, specifically, the octet rule. For each molecule the participant constructs, they are first presented with possible shapes for that molecule. Next, the participant virtually constructs this molecule using simulated model atoms. When building, the simulation logic reinforces realistic forces with respect to VSPER theory, so a disturbed "bonded" atom will return to its previous position. As shown in Figure 1, the simulation only allows user to construct the water molecule with a realistic bent shape: if atoms are moved out of position, they will return back to the true shape. We visualize the two sets of electron lone pairs repelling the hydrogen atoms as marked by red lines as well as elongated orbitals. Including these electron clouds in the VLE allow users to understand the forces of these electrons as stated in VSPER theory.

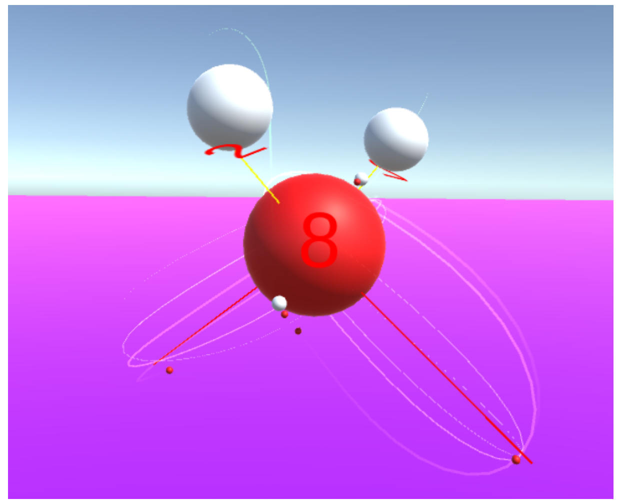

Fig. 1. Simulated water molecule. Two lone electron pairs take up space on the bottom side, resulting in a bent molecular geometry.

Figure 2 exhibits the result of a participant constructing Hydrogen cyanide(HCN) which demonstrates that our VLE provide specific visual queues to highlight to users the presence of a double or triple bond. Not only do we draw three sets of lines between the triple-bonded atoms, but we animate three of each atom's electrons (colored the same as their respective base atoms) orbiting around both atoms in the bond. These visual representations emphasise the affect double and triple bonds will have on resulting molecular geometry. Over previous iterations of testing, stressing these details proved crucial to the users ability to visualize molecular structures.

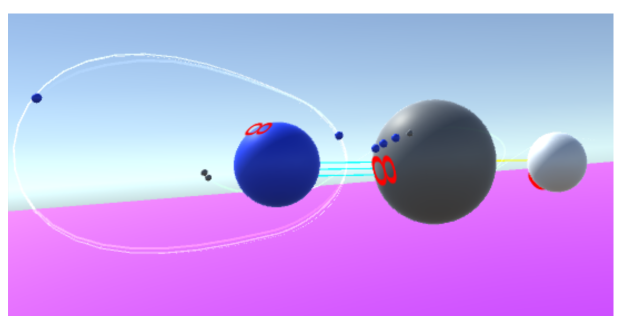

Fig. 2. Simulated hydrogen cyanide molecule with a triple bond between the nitrogen atom and the carbon atom.

2) *Simulation tasks:* We conducted three tasks in each of the nine scenes within our Virtual Reality application. Administering nine exercises was essential to distinguish molecular geometric patterns caused by the VSPER theory. Figure 3 exhibits an example of a scene layout with the base atom needed for the given formula as well as potential atoms for bonding,while Figure 4 displays four illustrations of possible atomic arrangements in which the users will reference to after assembling the molecule.

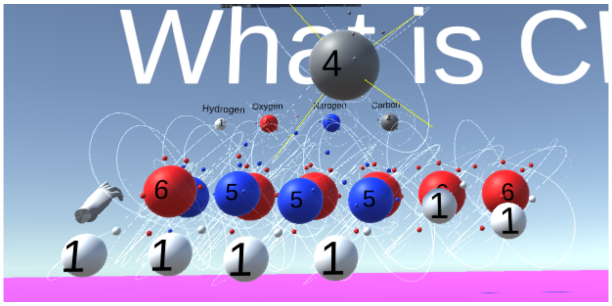

Fig. 3. Virtual learning environment capture. The participants are given a base atom with accessible bonding atoms below.

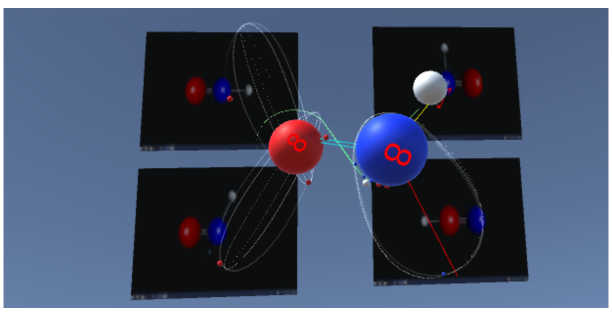

Fig. 4. Virtual learning environment capture. The participant observes possibilities for Nitroxyl molecule shape, then builds the molecule themselves.

Participants began each scene by first predicting the geometry of the specified molecule utilizing the four conceivable depictions as shown in Figure 4. Subsequently, the user would then construct the given formula wielding the allotted atoms. Lastly, they would relate the molecule to the correct configuration contemplating the type of connecting bonds and the lone pairs that contribute to the architecture of the model.

Through these assignments, participants demonstrated a more profound understanding of the patterns and concepts of orbital hybridization and VSPER theory. These interactive exercises engaged the users which is fundamental to comprehending abstract theories.

B. *Traditional Learning Experience*

To fully evaluate the effects of learning molecular geometry in our VLE, we collected data from a control group that use a traditional method of learning the VSPER theory. We provided them with a paper that explained the theory of electron repulsion and its affiliation to the geometric structure of a molecule as well as provided them with visuals of nine varying patterns identical to the ones in our VLE.

This control group reproduced a contemporary depiction of how chemistry classes relay topics of orbital hybridization through textbooks. Comparing this method of teaching to our VLE validates the use of Virtual Reality as a tool for learning.

C. *Questionnaire*

Each participant was required to complete a questionnaire before and after their respective learning experiences in pursuance of assessing their knowledge of molecular geometry with respect to the VSPER theory. For test subjects who engaged in our VLE, their level of immersion was additionally documented. The immersion questions took numeric responses from 0 - 4, with the key being “Not at all” (0), “Slightly” (1), “Moderately” (2), “Fairly” (3) and “Extremely” (4).

1) *Pre-Questionnaire:* A pre-questionnaire was conducted before the test subjects evaluated the concepts of the VSPER theory. This survey was directed to gain insight of the participants’ demographics and their prior knowledge of chemistry principles. Several inquiries were given asking to predict the molecular geometry of a simple molecule provided the electron count and chemical bonding types. Gauging the volunteer’s backgrounds and abilities eliminated potential biases or prejudice within our study.

2) *Post-Questionnaire:* Following their corresponding learning experience, each participant completed the post-questionnaire which consisted of three parts. A test subject answered ten questions to assess their comprehension of molecular geometry by using the VSPER theory, reported their perception of the difficulty of the chemistry questions, and if they engaged in our VLE, responded to questions of immersion both during and after our simulation.

Each of the ten chemistry question given presented a particular chemical formula resembling but different than the ones in the learning methods along with the involved atoms and the number of electrons in each outer shell. Four possible suggestions of the atomic configuration were displayed as well. This test served as a measurement of understanding of the abstract VSPER theory. Having ten questions with four options was crucial gauging their level of learning to reduce the degree of noise.

The next set in the post-survey allowed the test subjects to provide qualitative responses about the chemistry questions. Participants indicated the level of difficulty in the assessment of molecular composition retention. This section granted participants to express any confusion or opinions that help clarify our simulation or evaluation for future improvement. We omitted these questions from our analysis.

The immersion survey assessed the engagement of the Virtual Reality group during and after the experience. Recording these attributes allowed us to determine any correlation between the test results and captivation within our VLE.

III. Demographics

The pre-survey collected participant’s demographic information such as age group, location, gender, ethnicity, highest education, annual household income, and employment. Our test group consists of n = 69 participants with 42 in the experimental group using our VLE and 27 in the control group. 78.5% of the participants' primary field of study are engineering based with the majority focusing on computer science and electrical engineering. The additional statistics of the participants demographics are shown in Figure 5 The demographics were evenly distributed between the two groups.

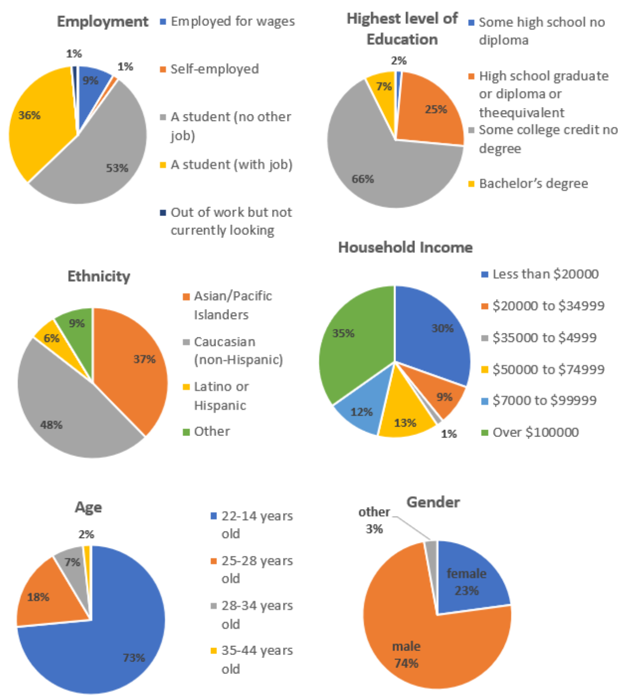

Fig. 5. Group demographics. The distribution of the participants age, level of education, employment status and ethnicity.

IV. Results

Virtual reality participants learned VSPER theory in our molecular simulation better the control group was able to learn via traditional learning methods. For every molecule in our simulation tasks, we showed the control group the same molecule with its realistic shape. Although the core of each educational experience we provided to was equivalent, participants that engaged our VLE grasped the concepts more intuitively. We observe this result by comparing the volunteers' scores.

Each of the ten post-questionnaire questions evaluate each participant's ability to apply VSPER theory to predict the resulting molecular shape of novel molecules. Participants, after engaging our VLE, were able to correctly answer eight of these questions on average. Yet the 27 participants that instead saw the same molecules but did not have the experience of constructing them in our VLE averaged five and a half of these questions correct. Our results suggest individuals can better assimilate the VSPER theory in a virtual learning environment.

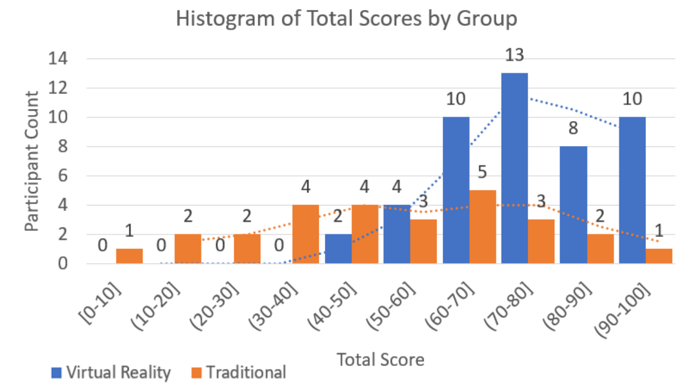

Fig. 6. Histogram of post test scores for both traditional (orange) and Virtual Reality Participants (blue): Participant count vs total score.

A. Total Scores

Figure 6 presents a histogram of the scores of each participant by test group. The most common score for the players that engaged our VLE was 8 of 10 correct questions, with an average score of 81.7%. Although the most common score for control group members was only one correct answer fewer (7 of 10 questions correct), these scores exhibited a higher variance. Control participants' average score was 55.9%, with a standard deviation of 24.2% (2.42 correct answers). For comparison, we calculate standard deviation of our VLE participants to be 14.3% (1.43 correct answers).

We interpret the lower average score and increased variance of the control group as evidence of superior understanding of VSPER theory for those that participated in our VLE. Participants, after engaging with our VLE, could correctly apply VSPER theory in 2.57 more questions, on average, than members of the control group. In this way, post-VLE participants better understood VSPER theory and its use to predict a molecule's geometry: their scores average 25.7% above control group average score.

We also interpret the distribution of these scores, not just their averages. As shown by the histogram, the standard deviation of the control group's scores is nearly double that of the scores from post-VLE participants. In our analysis of this statistic, we assume both group's volunteers began the study with similar preconceptions of valence electron theory and its affect on molecular geometry. Thus, we infer that engaging with our VLE helps participants establish a baseline of understanding, while a less effective educational experience would struggle to build upon these dramatically varied preconceptions. Our interpretation of the scores between the two groups suggests a superior learning outcome in participating with a VLE than with engaging with similar material in a traditional method.

B. Average Score by Question

1) All Participants: Figure 7 compares each group's frequency of correct answers for each question. By comparing each question individually, we show that engaging in our

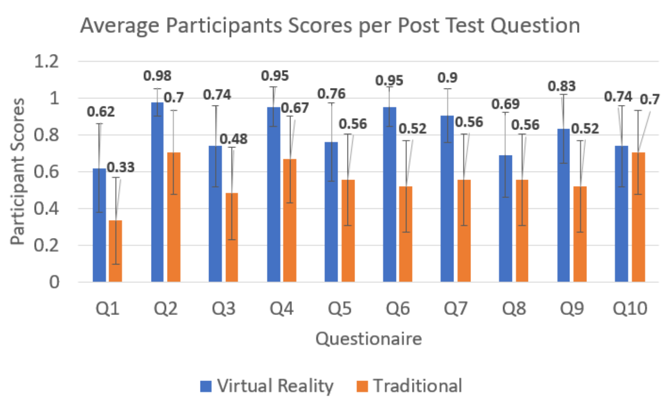

Fig. 7. Post Questionnaire results for both Virtual Reality group (blue) and non Virtual Reality group(orange): Participant scores vs Questions.

VLE improves a participant's ability to correctly answer each question. For the average question, participants that engaged our VLE were 25.7% more likely than members of the control group to choose the correct answer.

Yet, as shown in Figure 7, using the VLE did not help participants equally for each question. Interestingly, the virtual learning environment especially helped users correctly answer the sixth question of the post-questionnaire. Question 6 tested the participants on carbon disulfide (CS2) which consists of two double bonds. This particular molecule contains a similar structure to carbon dioxide (CO2) which was presented in both the VLE as well as traditionally on paper. The Virtual Reality group appeared to recognize the bonding effect pattern more intuitively than the the control group. 95.2% of post-VLE participants correctly identified the molecular geometry of carbon disulfide (the molecule from Q6), yet only 51.9% of control group participants could do this correctly. Thus, we conclude that participants that engage with our VLE are 43.4% more likely to be able to correctly apply VSPER theory to predict the molecular geometry of a linear molecule with two sets of double bonds.

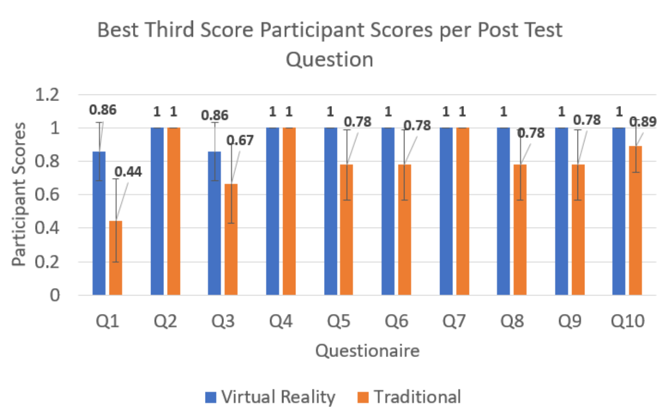

Fig. 8. Post Questionnaire results for the best third score for both the Virtual Reality group (blue) and non Virtual Reality group (orange): Participant Scores vs Questions

2) Best Participants: Figure 8 shows average correctness by question, but for only the highest-scoring third of their respective groups. We again observe that participants, after using our VLE, understand the material better and correctly answer questions more frequently than control participants. In fact, the top third of our VLE group had perfect correctness on eight of ten questions.

Notably, the top third of the two groups differed dramatically in their ability to correctly answer question one. Question one asked participants to predict the molecular geometry of Hydrogen Sulfide, given its chemical formula and those atom's respective numbers of valence electrons. Hydrogen sulfide has similar molecular geometry to water; we infer that post-VLE users are better able to apply VSPER theory in this question after interacting with a virtual water molecule in our simulation.

C. *Immersion Responses*

The last element of our post-questionnaire used two surveys to evaluate the degree of immersion of the VLE experience during and after our interactive simulation. Each question in the assessment related to specific categories in order to efficiently calculate the effects of engagement.

Our first survey categorized immersion responses which participants reported about their experience while engaged in the VLE. We used seven of these categories (competence, sensory and imaginative immersion, flow, tension and annoyance, challenge, negative affects, and positive effects) and for this immersion feedback. For the second survey, which collected immersion responses relating to post-engagement, we used six components (basic attention temporal dissociation, transportation, challenge post, emotional involvement, and enjoyment).

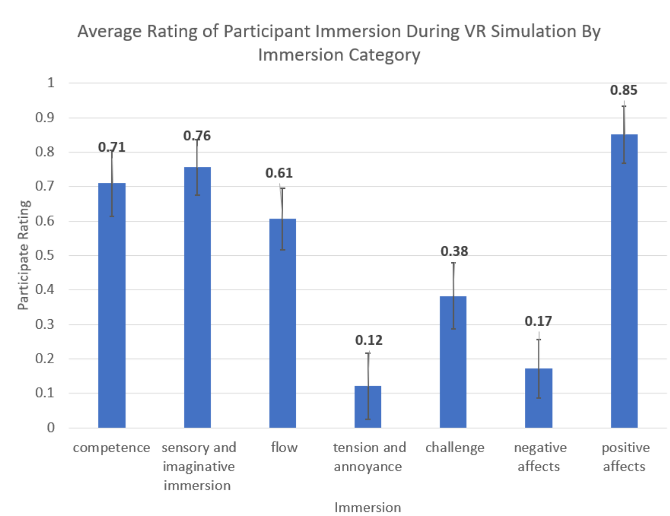

Fig. 9. Average Immersion feedback from participants during the simulation

Figure 9 displays the evaluation of the participants' VLE experience with in our simulation. Each component is ranked from a number between 0 and 1, where 0 indicates total disagreement and 1 total agreement. The results of immersion show that the average participant was highly immersed in the simulation. Although they indicated slight challenges, this did not promote frustration or an adverse mindset establishing a successful setting for a positive and engaging learning experience for the users.

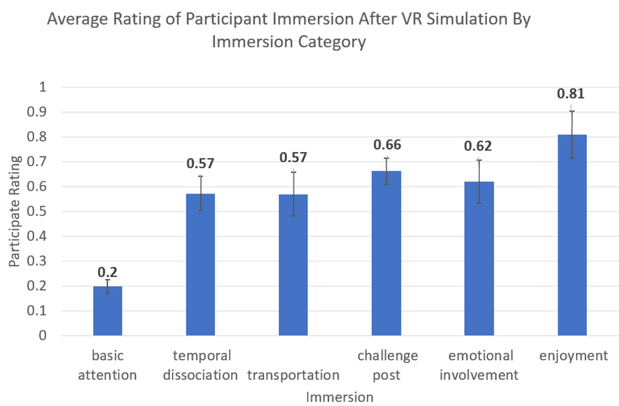

Fig. 10. Average Immersion feedback from participants after the simulation

The immersion feedback from participants after the simulation can be evaluated from Figure 10. Our post-engagement survey aims to consider the affiliation between learning outcomes and levels of attention and perception. Participants reported a low level of attention, so we interpret that enjoyment and transportation are more important immersion categories that brought about our educational results.

D. Immersion Correlations

In investigating correlations between immersion survey results and correctness in applying VSPER theory, we looked specifically for these correlations in question ten correctness. Figure 7 shows a near-negligible difference in correctness frequency for chemistry question ten. If the average post-VLE participant struggled in applying VSPER theory to this question as much the average control participant, then perhaps the most immersed VLE participants would perform better on this question than participants reporting less immersion.

The participants who correctly applied VSPER theory on question 10 had an overall more positive experience than those who scored worse. Figure 11 shows that users who could correctly answer this question reported a greater level of competence, sensory immersion, flow, and positive effects, on average.

V. Conclusion and Future Work

Through our research, we have determined that using VLE simulation to teach VSPER theory achieves better learning outcomes than traditional methods of teaching VSPER theory. In particular, the learners using our VLE achieved higher comprehension of the VSPER theory and an ability to predict molecular geometry. We also found a correlation between

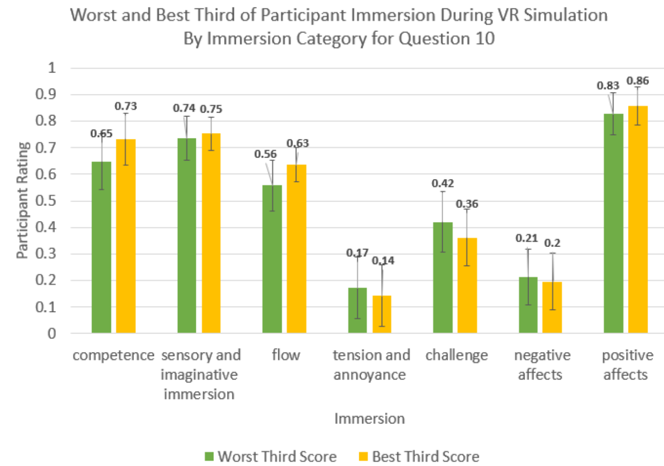

Fig. 11. Immersion feedback from participants during the simulation for question 10 for both the worst third score (green) and the best third score(yellow): Participant Rating vs Level of Immersion

higher levels of immersion and the level of understanding of the theory.

Our promising results of immersion and comprehension for simple molecules encourage our study to incorporate more complex structures. Planned future work includes to development configurations of carbon chains in our VLE to support interactive visualization for carbon molecules and enhance the learning of molecular geometry for organic chemistry.

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