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3D VIRTUAL REALITY FOR ENHANCED VISUALIZATION IN ORGANIC AND BIOORGANIC CHEMISTRY EDUCATION: ADVANTAGES, DISADVANTAGES, CHALLENGES AND SOLUTIONS

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The convergence of 3D virtual reality (VR, a simulated experience that uses pose tracking and near-eye 3D mapping to give the user a sense of immersion in the virtual world), and augmented reality (AR, interactive experience when a real-world environment is enhanced with computer-generated stimuli) in the educational landscape of Organic and Bioorganic Chemistry holds the promise of revolutionizing the learning experience, offering students a robust platform to explore and comprehend molecules and chemical reactions [1]. This symbiosis includes a variety of **benefits**:

Molecular Visualization. Researchers can harness VR capabilities to delve into the complexities of molecular architectures, enhancing their understanding of the spatial organization of atoms within organic compounds [2, 3]. Three-dimensional visualization enhances the perception of spatial arrangements, especially stereochemistry, which is crucial for comprehending Organic Chemistry concepts.

Interactive Learning. The interactive features of VR enable students to actively manipulate molecular structures, explore intricate reactions, gain insights into reaction mechanisms, intermediates, product formations, and witness real-time consequences, fostering a dynamic and engaging learning environment [4, 5]. This hands-on experience can deepen their understanding of Organic Chemistry principles.

Virtual Laboratories. Simulated labs establish an interactive environment where students and researchers can engage with virtual apparatuses, conducting experiments in a secure and controlled setting while employing critical reasoning [6, 7].

Collaborative Research. VR platforms facilitate real-time collaboration among researchers situated in disparate locations. By sharing three-dimensional models of molecules and engaging in discussions within a virtual space, researchers can enhance collaborative efforts and the transparency of communication [8].

Engagement and Motivation. Exploring chemical structures in a virtual environment with the incorporation of gamification elements, such as visual novels, makes the subject matter much more captivating [6–10].

Professional Development. Training modules and simulations can assist chemists and researchers in enhancing their skills and staying abreast of new methodologies [11].

Teacher Effectiveness: VR supports increased student engagement, automated grading, efficient time management, and the ability to illustrate educational processes using multimedia [3].

Adaptability to Personal Needs: VR programs can be tailored to accommodate various skill levels, learning styles, and the diverse needs of students with disabilities, spanning from foundational concepts to advanced topics [12].

Experimentation in a Safe Environment: Virtual laboratories allow students to conduct experiments in a simulated environment, providing a valuable resource for practicing techniques safely before entering a physical laboratory [13]. This is especially useful in secure remote settings, such as virtual learning at a distance (e-learning), during war or quarantine [6].

While VR presents numerous advantages for enhancing the learning experience in Organic Chemistry, there are also noteworthy **potential disadvantages** to consider:

Cost and Accessibility. Not all educational institutions may have the budget to invest in such technology, pay for its license usage [14], or expenses that exceed the cost of other equally effective training methods [15].

Technical Requirements. Ensuring that students have compatible devices may pose challenges, especially if there are disparities in the quality and capabilities of available hardware [15].

Limited Quality Content Availability. The range and depth of available VR educational materials may vary across different topics [1]. Nevertheless, traditional teaching methods can enrich the discussion on the adoption of VR in Organic Chemistry education.

Health Considerations. Some individuals may experience motion sickness or discomfort [16, 17], when using VR glasses, particularly during extended sessions, or/and negative rumination (i.e., harmful self-related thoughts related to distress) [18].

Isolation from Reality. While VR can simulate laboratory environments, it doesn't replicate the tactile and sensory experiences of traditional lab work [19].

Potential for Distraction. There is a risk of students becoming more focused on the novelty of the technology than the educational content [19].

Digital competence. Students and educators may need more time to familiarize themselves with VR technology due to different levels of digital competence and proper pedagogical aspects of its usage [16, 20].

Dependency on Technology. Technical glitches or malfunctions, such as software crashes or hardware failures, can disrupt the learning experience [14].

Proper validation: Additionally, the effectiveness of VR-based education should be validated through research and pedagogical assessments [16, 21] to ensure it enhances learning outcomes.

So, VR can be employed to create immersive environments for molecular docking simulations, namely engage in interactive sessions exploring the binding interactions between ligands and receptors, gaining insights into structure-activity relationships [22]. This is particularly relevant in the context of Bioorganic Chemistry, Drug Design and Pharmaceutical Chemistry. Here are a few **websites** that have contributed to providing **3D visualization** of organic structures, namely:

MolView [23]. It is a web-based platform that allows users to visualize and interact with chemical structures in 3D. It is designed for educational use and offers various tools for exploring molecular models.

ChemTube3D [24]. It provides interactive 3D models of various chemical compounds, including organic molecules. It is a free resource designed to aid in the teaching and learning of chemistry.

Virtual Chemistry 3D [25]. It proposes 3D animations and structures, with supporting information for some important topics covered during an undergraduate chemistry degree and beyond that.

MolecularVR [26]. It focuses on creating virtual reality experiences for molecular visualization. While it may not be exclusively for educational purposes, the immersive nature of VR can enhance the learning experience.

Hence, it should be considered that designing and programming a synthetic engine for 3D-VR generation in organic synthesis presents various challenges due to the complexity of the chemical reactions and the immersive nature of the VR experience [1, 3, 7, 15, 27, 28]. Thus, **key challenges** and their **solutions** when using VR in chemical sciences are as follows:

Development Resources. Establish partnerships with educational institutions to access a pool of skilled developers, chemists, and educators. Collaborate with professional organizations related to pharmaceuticals and chemistry for expert input.

Accurate Molecular Visualization. Employ advanced molecular visualization software and techniques to ensure precise 3D representations. Regularly update the program with the latest advancements in molecular visualization technology.

Reaction Complexity. Provide a comprehensive database within the VR program, detailing various reactions, conditions, reagents, and mechanisms. Incorporate guided tutorials and step-by-step walkthroughs for complex reactions.

Realism and Authenticity of Laboratory. Collaborate with laboratory experts to ensure accurate depictions of settings, equipment, and reactions. Regularly update the program with new equipment and realistic reaction scenarios.

Interactivity. Implement user-friendly controls for manipulating molecular structures and changing reaction conditions. Integrate tutorials and hints to guide users through interactive elements, ensuring a smooth learning curve.

Data Integration. Develop an adaptive algorithm that adjusts the program based on user inputs and learning progress. Provide dynamic data overlays to enhance the understanding of molecular structures and reactions.

Technical Limitations. Ensure compatibility with a broad range of VR hardware and software platforms through regular updates. Optimize connection stability by addressing potential issues related to VR devices and Wi-Fi routers.

User Experience. Conduct user testing and gather feedback for iterative design improvements. Prioritize simplicity and clarity in interface design, ensuring a smooth and intuitive user experience.

Assessment and Feedback. Implement real-time feedback mechanisms to inform users of the consequences of their actions. Include assessment tools and quizzes to reinforce learning and provide measurable progress.

Iterative Testing. Establish a continuous feedback loop involving students and educators for ongoing improvements. Conduct regular evaluations to assess the educational effectiveness and make necessary adjustments.

In summary, the ongoing technological evolution and the growing integration of VR and AR in scientific domains have the potential to give rise to innovative applications that may substantially influence different aspects of Organic and Bioorganic Chemistry education within this rapidly advancing field.

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