

## Immersive Virtual Reality and Computational Approaches for Advancing Chemistry Education: A Narrative Review

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### Abstract

This narrative review explores the integration of virtual reality (VR) as a transformative instructional medium in computational chemistry, focusing on how VR can address challenges such as limited 3D visualization and costly experimental setups. VR tools like iMD-VR and Nanome offer immersive interaction with 3D molecular structures, enhancing both conceptual understanding and practical skill development. By fostering engagement, critical thinking, and confidence among learners, VR makes complex chemical phenomena more accessible. However, infrastructure limitations and insufficient empirical data persist, especially in resource-constrained regions. Recent studies emphasize cloud-based solutions and collaborative VR labs to reduce costs and improve scalability. This review highlights VR's potential to modernize chemistry education, calling for more rigorous research to validate its long-term impact on learning outcomes.

**Keywords:** Virtual Reality (VR); Computational Chemistry; Chemistry Classroom; Molecular Structure

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## INTRODUCTION

Computational chemistry applies theoretical chemistry through programming to study molecular properties and behaviors, enabling real-world applications. Merging VR with computational chemistry can strengthen molecular visualization, enhance discovery, and improve chemistry education. As Papadakis et al. (2023a) emphasize, leveraging cloud-based solutions alongside VR can foster open, scalable learning and support data-intensive analysis. Thus, the adoption of VR as an educational medium introduces new technical skills—from handling 3D models to managing advanced data via cloud platforms—making complex analyses more feasible. VR has rapidly advanced in the last decade (Luckerson, 2014) and presents a novel avenue for transforming chemistry instruction.

The visualization of VR technology constructs immersive virtual environments, facilitating real-time, multimodal interaction (Cipresso et al., 2016; Di Lernia et al., 2018; Freeman et al., 2017; Neri et al., 2017; Riva, 2018). Such 3D spatial resolution and flexible manipulation of molecular structures (Feiner et al., 1997; Schmidt et al., 2017) heralds a new era in chemistry education. For instance, the interactive MD in VR

(iMD-VR) leverages the DFTB+ code and showcases VR's capacity to enrich teaching (Deeks et al., 2020). In line with Papadakis et al. (2023b), coupling VR with cloud-based simulations further expands the potential for multi-user collaboration and real-time data sharing, reinforcing deeper student engagement.

While some question VR's feasibility, successful applications in organic chemistry validate its potential in science education. For instance, Ferrell et al. (2019) deployed iMD-VR as a teaching medium, improving the quality of organic chemistry instruction. Typically, VR kits include controllers and wearables that let users touch, drag, or rotate molecular structures, enabling hands-on engagement. As Papadakis (2020) notes in the context of computational thinking, early exposure to interactive technologies can cultivate advanced analytical skills—a principle that extends naturally to VR-based chemistry exploration. This tactile immersion helps learners grasp 3D concepts with greater clarity than traditional methods.

Moreover, students can navigate a 360-degree virtual environment via head-mounted displays, offering an immersive alternative to screen-based interaction (Fombona et al., 2020; Pastel et al., 2022). Nevertheless, the lack of rigorous, long-term studies on VR's effectiveness in chemistry education remains problematic (Dunnagan et al., 2020; Scavarelli et al., 2021). Papadakis et al. (2023a) highlight the importance of systematic evaluation to ensure consistency, equity, and efficacy when deploying novel technologies. Despite these research gaps, VR's potential to transform educational practice—by enhancing engagement, interactive learning, and deeper conceptual understanding—warrants further exploration in diverse chemistry classrooms.

## METHOD

This study employed a narrative review approach to investigate the integration of virtual reality (VR) and computational techniques in chemistry education. This format was chosen due to the broad scope of the inquiry, which encompasses a range of VR platforms, diverse educational contexts, and varied student demographics (Daemi et al., 2021). Unlike a systematic review or meta-analysis, this narrative review aims to synthesize overarching themes, pedagogical insights, and emerging innovations (Cummins et al., 2024; Hall et al., 2021) rather than quantitatively aggregating effect sizes.

By integrating thematic breadth with contextual depth, this narrative review offers a comprehensive overview of how VR merges with computational chemistry to transform teaching and learning practices. The method's flexibility allowed the inclusion of a wide range of studies—from empirical work to conceptual explorations—thus reflecting the rapidly evolving and interdisciplinary nature of VR in chemical education.

## Scope and Objectives

The primary objectives were to (1) explore how VR-based interventions enhance learning outcomes in chemistry, focusing on engagement, conceptual understanding, and cost-effectiveness; (2) examine computational tools (e.g., molecular modeling, MD simulations) used alongside VR, highlighting how these techniques deepen students' grasp of complex chemical phenomena; and (3) identify practical challenges (cost, technical expertise, infrastructure) and propose avenues for addressing these barriers.

## Literature Search Strategy

A comprehensive search was conducted using Scopus, Web of Science, and Google Scholar (see Table 1). To broaden the literature base, relevant conference proceedings and preprint servers were also scanned. The following terms were combined with Boolean operators (AND/OR) to capture the breadth of VR applications in chemistry education.

- "Virtual Reality" OR "VR"
- "Chemistry Education"
- "Computational Chemistry"
- "Immersive Learning" OR "3D Visualization"
- "Molecular Modeling" OR "MD Simulation"

**Table 1.** Summary of the Search Strategy

Element	Details
Databases	Scopus, Web of Science, Google Scholar
Search Terms (Examples)	"Virtual Reality," "Chemistry Education," "Molecular Modeling," "MD Simulation," "Immersive Learning"
Search Period	Primarily 2018–2023 (extended if seminal works were identified in references)
Inclusion	VR-based studies, computational tools in chemistry, empirical or review articles, English-language publications
Exclusion	Non-peer-reviewed or purely theoretical papers (no direct educational context), VR for non-chemistry fields without relevance
Screening Levels	Title & abstract screening → full-text review → data extraction & thematic grouping
Additional Sources	Reference tracking (snowball sampling), institutional repositories, relevant conference proceedings

## Inclusion and Exclusion Criteria

The following criteria guided the selection of studies for this narrative review. Emphasis was placed on identifying research that specifically investigates the application of VR in chemistry education and highlights its integration with computational or simulation-based tools. Table 2 summarizes the key inclusion and exclusion elements considered at each stage of the screening process.

**Table 2.** Inclusion and Exclusion Criteria

Criteria	Description
<b>Inclusion</b>	<ul style="list-style-type: none"> <li>• Studies focusing on VR or immersive technologies with a direct application in chemistry education (e.g., simulations of molecular structures, lab exercises, or chemical analysis).</li> <li>• Empirical (quantitative or qualitative) or theoretical works that provide pedagogical insight (e.g., assessing student engagement, performance, conceptual understanding).</li> <li>• Articles exploring computational chemistry or simulation tools integrated with VR (e.g., MD simulations, quantum modeling) to deepen learning outcomes.</li> </ul>

Criteria	Description
<b>Exclusion</b>	<ul style="list-style-type: none"> <li>English-language papers published in peer-reviewed journals, conference proceedings, or high-quality academic repositories.</li> <li>Publications focusing solely on VR outside the chemistry domain (e.g., engineering, medicine) without clear relevance to chemical concepts.</li> <li>Sources lacking sufficient methodological detail on how VR was applied or evaluated (e.g., purely theoretical frameworks without educational data).</li> <li>Non-peer-reviewed materials or gray literature with limited substantiation (e.g., blog posts, newsletters).</li> <li>Research that does not address student learning, engagement, or performance in a chemistry-specific context.</li> </ul>

These criteria helped ensure that the review captured a comprehensive range of relevant VR-based studies within chemistry education, while filtering out materials lacking clear methodological or pedagogical significance.

### Screening and Selection Process

Using the keywords listed in Table 1, results were compiled and exported to a reference management tool. Duplicate records were removed, and remaining items underwent title and abstract screening for relevance. Potentially eligible papers were then reviewed in full, ensuring they met the inclusion criteria. Relevant references within these papers were assessed (snowball sampling) to capture additional material. Any discrepancies in study selection were resolved through discussion among the authors.

### Data Extraction and Thematic Analysis

Key details—such as study design, VR technology used, computational tools, sample demographics, and primary outcomes—were extracted into a shared spreadsheet. Studies were organized by thematic categories (e.g., “molecular visualization,” “experimental simulations,” “learner engagement”), enabling a structured comparison of findings. Qualitative insights (e.g., student feedback, classroom observations) were also integrated to capture the multifaceted impact of VR in chemistry education.

### Review Limitations

Because this review is narrative rather than systematic, it does not strictly adhere to protocols like PRISMA, and findings may be subject to publication bias or variability in study quality. Additionally, VR technologies evolve rapidly, so certain reported outcomes might become outdated or superseded by newer hardware and software.

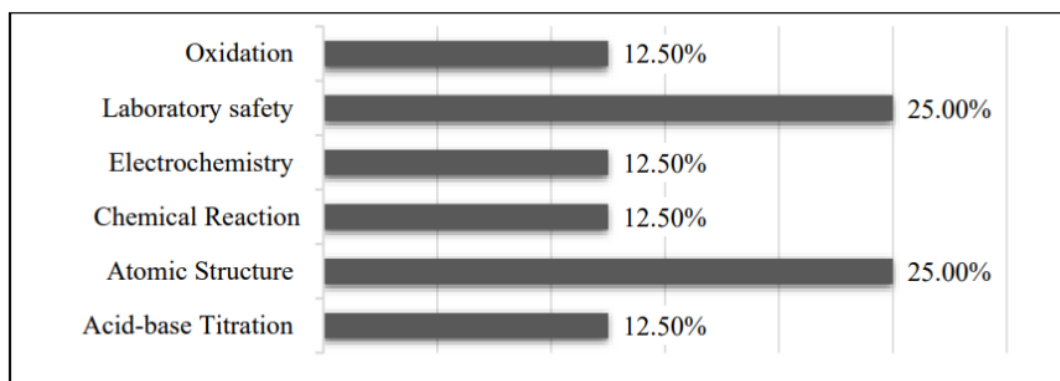
### Ethical and Quality Considerations

All analyzed sources were publicly available and peer-reviewed, avoiding the need for institutional ethics approval. Emphasis was placed on each study’s design rigor—sample size, methodology, and outcome metrics—to ensure that insights discussed are grounded in well-documented educational research.

## RESULTS AND DISCUSSION

### Virtual Reality (VR) in Chemistry Education

Different studies were conducted to investigate the integration of virtual reality laboratories (VRLs) in the Chemistry subject, with databases (Scopus and Web of Science) accessed for data collection. From the results, many articles published between 2018 and 2022 promoted Virtual Reality Laboratory (VRL) in chemistry (Guruloo & Osman, 2023). Most of the research found that laboratory safety and atomic structure were the popular topics discussed, as shown by the percentage of Topics of Integrating VRLs in Chemistry Education (Figure 1). Various technological tools are used to integrate VRLs into chemistry education. The Oculus system was the most common, making up 50% of tools used in VRLs; other VRL technologies include Sim View (12.5%), real-time systems (12.5%), VR simulations (25%), Narupa XR (12.5%), and Google Chromecast (12.5%). While VRLs show immense promise for transforming chemistry education, this technology requires expertise, costly equipment and software, as well as well-trained educators. Papadakis et al. (2023b) emphasize that combining VR with cloud-based frameworks could mitigate some of these infrastructural barriers, making VRLs more accessible.



**Figure 1.** The percentage of Topics of Integrating VRLs in Chemistry Education. Picture was obtained from (Guruloo & Osman, 2023)

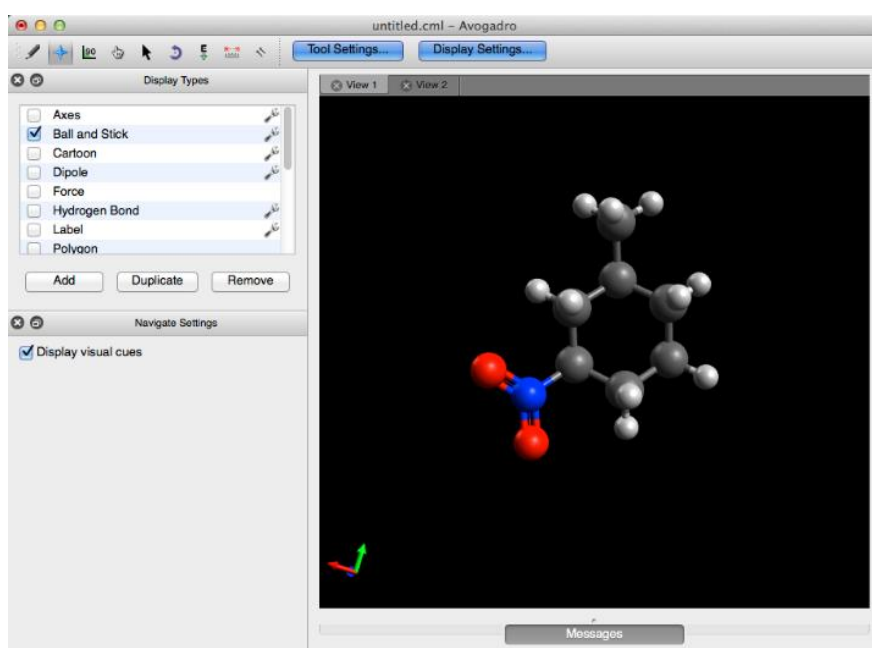
### Enhancing Visualization: 2D vs 3D Approaches

Many programs enable molecular visualization on 2D screens, though they lack the immersive feature of VR. Most of these programs use 3D simulations via desktop software, but do not incorporate stereoscopic vision (virtual reality). Despite this limitation, 2D visualization tools allow chemists to perform a range of tasks, including molecular mechanics calculations, visualizing molecular orbitals and surfaces, and animating normal vibration modes and spectra. Additionally, this 2D technology supports reading various file formats (e.g., PDB, Mol, XYZ, CIF) and generating videos (MP4) or images (PNG), ensuring continuous applicability in molecular visualization and data analysis. Research has demonstrated the significant advantages of using interactive visualizations as instructional resources to aid students in the learning process (Ryoo et al., 2018). Papadakis (2020) further suggests that cloud-based or mobile platforms, when paired with immersive techniques, can enhance collaborative and interactive experiences.

These teaching concepts require three-dimensional explanations—particularly in Organic Chemistry (Edwards et al., 2019). Molecular representations in these



visualizations provide detailed insights into atomic structure, orbitals, electronic density, and other bonding properties. These models allow students to interact dynamically through computers using mouse, keyboard, and trackpad, enhancing accessibility while offering deeper conceptual understanding. Many popular software programs, such as Avogadro and Gaussian, include advanced features like Quantum Mechanical or Molecular Mechanical (QM/MM) calculations and Density Functional Theory (DFT) simulations. However, studying a molecular system typically involves preparing an input file to define the system, then analyzing the resulting data from computations. To facilitate molecular editing and visualization, various programs are often combined. PyMOL (Figure 2), for example, can be integrated with PyLabor NumPy for enhanced functionality (Romeo et al., 2020). Avogadro and Gauss View also contribute to molecular modeling, which is crucial for addressing fundamental research questions.



**Figure 2.** 3D visualization of viewing molecules. Picture was obtained from [avogadro.cc](http://avogadro.cc)

Traditional 2D tools can limit comprehension of macromolecular structures, but VR resolves this through immersive 3D representation (Berkmen et al., 2024). The Nanome VR app with Meta Quest headset aids students in visualizing and manipulating these complex structures. Through guided tutorials in Nanome, users can identify molecules, locate active sites, and edit protein structures. Student feedback indicated that 85% became more interested in protein structure after these hands-on VR activities, highlighting VR's capacity to make molecular learning more engaging and effective. However, VR does have its limitations, such as cost and technical setup. Chemistry and biology students commonly employ 2D molecular visualization tools like Avogadro and Gaussian for QM or DFT calculations, but these methods necessitate additional setup and lack true immersion. VR apps such as Nanome, conversely, let learners directly interact with 3D models, simplifying the understanding of bonding and complex structures. Emerging work from Papadakis et al. (2023b) suggests that cloud-based VR could further expand collaborative opportunities and reduce local hardware constraints.

### The Role of Virtual Reality in Chemistry Experimental Teaching

Chemistry experimental teaching applies classroom knowledge in hands-on activities, enabling students to understand chemical behavior and properties. Beyond imparting knowledge, real lab settings foster creativity, teamwork, problem-solving, social responsibility, and information literacy. However, traditional experimental teaching often faces safety issues, limited facilities, time constraints, and high costs for chemicals or equipment. In resource-limited contexts, VR labs present a cost-effective alternative to experiential chemistry education (Li et al., 2023). By creating interactive and realistic environments, VR enables students to conduct virtual titrations, molecular docking, or chemical reaction simulations (Figure 3) without incurring physical risks or excessive expenses. This safe, virtual approach lets students independently explore data, refine critical thinking, and practice chemistry lessons. Papadakis et al. (2023a) contend that integrating VR with cloud platforms could further enhance these practical experiences, offering collaborative, scalable lab simulations for diverse student groups.



**Figure 3.** VR-based virtual labs develop student's creativity and critical thinking without thinking about the risks. Picture was obtained from ixrlabs.com

### Bridging the Gap Between Hands-On and Virtual Learning: Lessons from Global Case Studies

The COVID-19 pandemic prompted sudden and significant changes to teaching practices, forcing educators to rapidly adapt to remote learning. Governments worldwide enforced measures that impacted everyday life. China, the first country to detect the virus's spread, saw widespread school closures and a shift to online formats (Omar et al., 2023). Likewise, in Malaysia, schools were closed in March 2020, affecting the education of five million students. To ensure continued learning, the Ministry of Education launched a nationwide online platform, assisting millions of students throughout these closures and remaining pivotal as schools gradually reopened from June 2020 (Kamal, 2020). Papadakis et al. (2023b) note that virtual environments can complement such emergency strategies, bridging gaps in both infrastructure and learning continuity.

Virtual Reality (VR) learning is increasingly adopted in Asian countries, particularly in engineering, chemistry, medicine, and vocational fields, as VR enables students to visualize complex concepts and simulate experiments. In Malaysia, 360-degree real-life video and VR technologies were used for remote teaching, especially

to improve communication skills among technical and vocational students (Adnan, 2020). A study conducted from 2019 to early 2020 involved 560 undergraduates—primarily from technical and vocational backgrounds, with a 40% male and 60% female ratio. During this phase, students experienced ELSA 360° video (Figure 4), a tool aimed at enhancing English and language proficiency. In the second phase, students participated in group discussions to provide deeper insight into their VR learning experience. Such immersive platforms exemplify how VR can expand learning beyond traditional classroom boundaries, offering authentic and engaging experiences.



**Figure 4.** ELSA 360° Video. Picture was obtained from Yusof et al., (2019)

The findings revealed that immersive tools like ELSA 360° possess significant potential to enhance learning experiences by developing communication, professional, and problem-solving skills. Using VR could thus benefit a wider range of academic subjects, including more challenging disciplines. However, the high data usage, cost of mobile data, and poor internet connectivity stood out as major barriers to equitable access. Despite these hurdles, Gungor et al. (2022) observed that students maintained strong interest, self-concept, and self-efficacy, alongside reduced lab anxiety. In a northern European university, 17 pharmacy students took part in a three-week organic chemistry course (2021), beginning with a VR practical using the Oculus Quest™ and an app built on Unreal Engine 4. This setup let instructors monitor VR sessions on an external display via Google Chromecast. Aiming to reduce lab anxiety and boost real-life lab efficiency, the app exposed students to building organic reaction setups in a fume hood. Early data suggest combining VR pre-labs reduces lab anxiety by about 30% and improves student preparedness. However, limitations include mismatched data and the novelty effect of VR as a relatively new educational tool.

Aalto University developed a virtual chemistry lab for nearly 200 chemical engineering students (Viitaharju et al., 2023). The virtual lab served as a pre-lab exercise to increase engagement and understanding without replacing hands-on experimentation. Students determined iron's mass and concentration in a commercial supplement using UV-vis spectrophotometry and flame atomic absorption spectrometry. Although students still preferred real-life chemistry labs—finding virtual ones repetitive—virtual labs present notable benefits, including interactive questions, gamified elements, and safe trial-and-error practice. Similarly, a virtual system was developed to simulate titration experiments before a physical lab, employing the Unity Real-Time Development Platform with Microsoft SQL Server



(Agbonifo et al., 2020). Results showed 60% found the virtual lab helpful, 66% said it was easy to use, and 54% strongly agreed it enhanced their learning. The Virtual Chemistry Laboratory (VCL) effectively supports acid-base titration comprehension prior to real-world lab sessions. Papadakis et al. (2023b) suggest that cloud-based solutions could further improve the scalability and collaborative aspects of such virtual labs.

These tools have shown noteworthy potential to boost student engagement, build skills, and lower anxiety, as evidenced by research in Malaysia, Europe, and beyond. As education systems continue adopting advanced technologies, tackling internet connectivity, cost constraints, and data requirements becomes essential for maximizing VR's potential. Papadakis et al. (2023a) emphasize that innovations in cloud and mobile technologies can further democratize access, ensuring equitable opportunities and improving learning outcomes across diverse educational contexts.

### **Recent Studies, Impact and Outcomes of Innovation**

Makransky et al. (2020) found that incorporating VR enhances student engagement, self-efficacy, and motivation to explore computational chemistry. Recent research highlights the crucial role of simulation techniques—especially at the atomic level—for predicting and modeling various material properties. Although learning new simulation tools can be daunting, students can select user-friendly or open-source platforms that align with their academic background and technical proficiency. Those new to MD simulations or computational workflows may consult comprehensive tutorials (Patel et al., 2022) to bridge initial knowledge gaps. For instance, CHARMMing (Jo et al., 2008) provides Langevin and MD simulations via an online interface, simplifying trial-and-error exploration for novice researchers. Similarly, SOCOT and ChemDraw remain invaluable in organic chemistry, enabling students to visualize reactants, track chemical transformations, and predict potential products. While many learners embrace these computational tasks with enthusiasm, others struggle due to the steep learning curve. Papadakis et al. (2023a) underscore that pairing VR with cloud-based simulation tools may further streamline the user experience, reducing hardware demands and lowering overall costs.

It is widely accepted that selecting the most appropriate software can optimize each program's unique strengths for experimental observations and simulations. Continuous training with a range of alternative tools not only broadens skill sets but also enhances problem-solving abilities in everyday scenarios. Recent empirical evidence underscores the effectiveness of Nanome—a VR platform—at significantly boosting student learning outcomes. In a quantitative study, Qin et al. (2021) observed that Nanome usage elevated students' performance to a 4.0 or higher on a 5.0 scale, suggesting marked gains in visualizing and understanding chemical structures. This instructional synergy addresses three central objectives: (1) empowering students to master novel technology skills, (2) enabling them to acquire higher-quality data for in-depth chemical analysis, and (3) fostering engagement and confidence through immersive, hands-on learning experiences.

In today's digitally connected environment, students commonly rely on smart devices for information—spanning from laptops to mobile phones and beyond. Consequently, introducing MD simulation and Nanome as instructional tools not only expands their technical proficiencies but also encourages the processing of complex

chemical data. Another vital objective is closing the gap between experimental data collection and contextual understanding. By using MD simulations and Nanome, students gain access to high-resolution insights at the atomic level, far exceeding what many traditional lab activities can deliver. These tools empower learners to autonomously analyze reaction pathways, electronic densities, and molecular dynamics with depth and precision. Ultimately, this method aims to stimulate student interest through an engaging, natural learning environment—thereby boosting confidence and reducing subject anxiety. As a result, recent evidence shows that Nanome, in particular, meaningfully enhances students' overall academic performance, confirming its viability as an effective VR aid in chemistry education.

## CONCLUSION

The integration of virtual reality (VR) into chemistry education has significantly transformed learning by providing immersive and interactive experiences that bridge the gap between theoretical concepts and practical applications. Virtual chemistry labs empower students to intuitively grasp molecular structures through direct manipulation, surpassing the limitations of traditional models. These VR methods enhance adaptability and deepen understanding of chemical mechanisms while reducing the reliance on 2D screens and manual programming. Moreover, the immersive aspects of VR cultivate student curiosity and make learning more dynamic, as complex content becomes more accessible and engaging. Despite ongoing challenges related to cost, technical support, and internet connectivity, VR platforms have demonstrated effectiveness in lowering student anxiety, improving performance, and promoting critical thinking. By continuing to advance pedagogical methods and refine virtual labs, VR can further ensure that students develop versatile skills, confidence, and a more profound appreciation for chemistry, thus preparing them for future scientific endeavors.

## RECOMMENDATION

Increasing the accessibility of VR in chemistry education calls for strategic measures that address both financial and infrastructural barriers. Institutions might explore cost-saving strategies such as forming partnerships with technology providers, implementing phased equipment rollouts, or adopting lightweight, open-source platforms. Tailored training sessions and ongoing technical support are equally important for ensuring that educators and lab instructors can effectively integrate VR into their teaching. Such support can include user-friendly guides, skill-building workshops, and a dedicated helpdesk to ease the transition for both instructors and learners.

Rather than fully supplanting hands-on laboratories, VR should enhance traditional experimental learning by offering additional virtual sessions that deepen students' conceptual understanding. This complementary use can broaden learners' perspectives while preserving essential practical competencies. In turn, longer-term assessments are valuable for clarifying the full impact of VR on educational outcomes, particularly regarding motivation, knowledge retention, and student confidence. Another way to strengthen these effects is to facilitate real-time collaboration in multi-user VR environments or through cloud-based solutions. Enabling group work in

virtual spaces can further develop communication and teamwork skills, which are fundamental for success in any scientific endeavor.

### Author Contributions

Conceptualization, KJ; validation, KJ, HFMZ, NFH; formal analysis, KJ, HFMZ, NFH; investigation, KJ, HMFZ, NFH; resources, KJ, HFMZ, NFH; writing—original draft preparation, KJ, HFMZ, NFH; writing—review and editing, KJ, HFMZ, NFH; visualization, NFH; supervision, KJ; project administration, KJ. All authors have read and agreed to the published version of the manuscript.

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