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# A VR-assisted hybrid teaching model for sustainable mechanochemical synthesis: educational overview and case study of a Cu–N-heterocyclic carbene undergraduate laboratory

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Integrating sustainable synthesis and modern instructional technologies into undergraduate laboratory education is essential for advancing chemistry teaching aligned with sustainability goals. This work presents an overview of the educational implications of virtual reality (VR) in modern education. It describes a hybrid teaching model implemented in an advanced undergraduate inorganic chemistry course, based on a survey of student preferences involving 109 students across multiple courses at Khalifa University of Science and Technology, United Arab Emirates. Using solvent-free mechanochemical synthesis and characterization of a copper N-heterocyclic carbene (Cu–NHC) complex as a representative example of contemporary, sustainable organometallic chemistry, the module integrates hands-on experimentation with immersive, transferable digital learning tools that can be used as teaching resources when access to mechanochemistry and nuclear magnetic resonance (NMR) instrumentation is limited. The VR-assisted session was implemented as a case study with a cohort of 15 undergraduate students who volunteered and focused on improving laboratory preparedness, procedural understanding, and familiarity with advanced synthetic and analytical techniques. Overall, this work demonstrates a feasible and scalable teaching model aligned with green chemistry principles and the United Nations Sustainable Development Goals.

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## Sustainability spotlight

Undergraduate chemistry laboratories are often resource-intensive, relying on large solvent volumes, extended reaction times, and restricted access to advanced instrumentation, which collectively limit sustainability and inclusivity in education. This work advances sustainable chemistry teaching by combining solvent-free mechanochemical synthesis with virtual reality (VR)-supported laboratory instruction. The hybrid teaching model reduces solvent use, chemical waste, energy demand, and laboratory time while preserving essential hands-on learning outcomes. By providing VR-based and computer-accessible (2D) instructional resources, the approach also improves equitable access to advanced techniques such as mechanochemical synthesis and NMR spectroscopy across institutions with varying infrastructure. This educational framework directly supports UN Sustainable Development Goal (SDG) 4 (Quality Education) through inclusive and modern pedagogy, and SDG 12 (Responsible Consumption and Production) by embedding green chemistry principles into experimental practice, offering a scalable model for sustainable laboratory education.

## Introduction

Sustainable and green chemistry strategies are increasingly employed to minimize or eliminate the use of hazardous

substances that pose risks to human health and the environment, in line with the United Nations (UN) Sustainable Development Goals.<sup>1,2</sup> In this context, the development and application of synthetic methodologies is no longer guided solely by efficiency and yield but also by environmental impact and resource sustainability.<sup>3</sup> Among these approaches, mechanochemical synthesis, where chemical reactions are driven by mechanical energy *via* ball milling or manual grinding, has emerged as a prominent and effective green technology.<sup>4</sup> Due to its solvent-free or solvent-minimized nature, mechanochemistry offers significant advantages over conventional solution-based methods, particularly by reducing energy expenditure and

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reaction times, as well as reliance on organic solvents, which constitute a substantial source of waste in large-scale pharmaceutical and fine chemical production.<sup>5</sup> In addition, mechanochemical activation can enable the preparation of indispensable functional materials that are difficult to access *via* conventional solution-phase synthesis.<sup>6</sup> These features align closely with the principles of green chemistry and the UN Sustainable Development Goals, positioning mechanochemistry as an attractive platform for environmentally responsible synthesis in both academic and industrial contexts. Notably, mechanochemistry was identified in 2019 by the International Union of Pure and Applied Chemistry (IUPAC) as one of the Top Ten Emerging Technologies in Chemistry, highlighting its safety and sustainability advantages.<sup>7</sup>

Mechanochemical techniques have proven particularly effective for the synthesis of transition-metal complexes with a broad range of applications, from active catalytic systems to advanced functional materials and medicinal chemistry.<sup>8–11</sup> For instance, Pd- and Cu-based complexes serve as indispensable catalysts in key transformations such as C–H activation and cross-couplings.<sup>12,13</sup> Beyond synthesis, mechanochemistry has also enabled greener, more operationally simple catalytic reactions with these complexes. Cross-coupling reactions are inherently sensitive to oxygen and moisture and often require inert atmospheres.<sup>14,15</sup> The application of mechanochemistry to such transformations benefits from eliminating solvent–catalyst interactions, accelerating reaction kinetics and reducing catalytic loadings while maintaining high efficiency. The enhanced kinetics, among other factors, can allow couplings to proceed under ambient air conditions, thereby removing costly inert gas constraints and making these reactions less energy-intensive and more practical for industrial and pharmaceutical applications.

Among metal complexes, Cu(I) N-heterocyclic carbene (NHC) complexes have attracted considerable attention across various fields, including carbene-transfer precursors, active catalysts, and medicinal applications.<sup>16–18</sup> Copper, as an earth-abundant and low-toxicity metal, combined with the strong  $\sigma$ -donating and robust coordination properties of NHC ligands, offers a cost-effective and environmentally favorable alternative to catalytic systems based on precious metals such as Pd and Ru. Cu–NHC complexes represent an essential class of compounds in organometallic chemistry, with broad relevance to catalysis and sustainable synthetic design.<sup>19–21</sup>

Given the increasing emphasis on sustainable and safer synthetic methodologies, integrating advanced materials and modern, greener synthetic approaches into undergraduate (UG) chemical education is becoming increasingly crucial. Experimental chemistry constitutes a fundamental component of the UG chemistry curriculum, providing students with essential practical skills, scientific training, and a deeper conceptual understanding of chemical principles through hands-on laboratory experience. These laboratory sessions play a critical role in reinforcing theoretical knowledge while fostering problem-solving abilities and experimental competence. However, UG teaching laboratories also present a range of safety concerns, including exposure to hazardous chemicals, handling fragile

glassware, and operating specialized equipment, all of which pose potential risks to student health and safety.<sup>22</sup> Implementing such laboratory sessions is often resource-intensive, requiring substantial time, financial investment, and infrastructure. Therefore, the development of alternative or complementary approaches that reduce these burdens while preserving educational value is highly desirable. Over the years, several strategies have been introduced to supplement laboratory-based instruction, including e-learning platforms, instructional videos, and digital simulations.<sup>23</sup> While these methods offer flexibility and accessibility, they frequently fall short in providing the level of interactivity and practical engagement necessary for effective experimental learning.

In this context, integrating virtual reality (VR) technology into chemical education presents a compelling opportunity to address these limitations. VR-based laboratory environments offer significant advantages, including enhanced safety, reduced costs, and greater time efficiency, while enabling students to engage with experimental procedures in a controlled, immersive setting.<sup>24</sup> Through immersive visualization, VR allows students to experience laboratory workflows that closely resemble real-life experimental conditions, facilitating visual learning and improving conceptual understanding. Moreover, VR has been shown to increase student motivation and engagement, thereby supporting more effective knowledge acquisition.<sup>25</sup>

Despite rapid advancements in VR technology across diverse disciplines, its adoption within chemistry education, particularly in laboratory instruction for the physical sciences, remains relatively limited. In this work, we present an overview of the educational implications of VR, along with a hybrid laboratory case study that integrates green mechanochemical synthesis with VR-supported instruction to advance undergraduate inorganic chemistry education. The design was informed by prior student feedback across multiple undergraduate courses and is supported by a set of reusable instructional resources, including VR videos that are also accessible in standard computer-based formats, to facilitate broad adoption across diverse educational settings. Using mechanosynthesis and characterization of a Cu–NHC complex as a representative example of modern, sustainable organometallic synthesis, the study combines solvent-free experimental practice with immersive, transferable digital learning tools. The hybrid framework is designed to enhance laboratory safety, sustainability, and student preparedness while preserving essential hands-on experimental skills, and is aligned with green chemistry principles and the United Nations Sustainable Development Goals. By building on recent literature in VR-supported education and mechanochemistry, this work illustrates a practical and transferable approach for integrating emerging instructional technologies into advanced undergraduate laboratory curricula.

## Educational and practical implications of VR

VR technology is being integrated into academic environments as a complementary tool to traditional teaching methods,



aiming to enhance student learning and engagement.<sup>26</sup> Fully immersive virtual environments, such as three-dimensional animations implemented using CAVE™ systems, have been shown to improve students' comprehension of molecular structures and reaction processes compared to conventional two-dimensional representations, while increasing motivation and engagement.<sup>27</sup> In chemistry education, simulations play a vital role by providing safe, repeatable environments in which students can explore chemical processes without risk, making them valuable for institutions with limited laboratory infrastructure and time constraints.<sup>28</sup> Such platforms also help students become familiar with real laboratory equipment and workflows before hands-on experimentation, increasing safety awareness.<sup>29</sup>

The advantages of VR-based interaction are especially evident in tasks requiring spatial reasoning and molecular manipulation. In studies where participants were challenged to perform operations such as threading a methane molecule through a carbon nanotube, altering helical screw sense, or manipulating protein knots, VR users consistently outperformed those using conventional interfaces. These improvements were attributed to enhanced depth perception, intuitive two-handed control, and improved molecular inspection afforded by immersive environments.<sup>30</sup> Winkelmann and co-workers demonstrated the effectiveness of the Second Life VR platform for conducting chemistry laboratory experiments in undergraduate General Chemistry courses.<sup>31</sup> Across multiple cohorts, students reported positive learning experiences, and comparative analyses of quizzes, laboratory reports, and practicum performance indicated that VR-based experiments were at least as beneficial as, and in some cases superior to, traditional laboratory instruction.<sup>32</sup>

Although the adoption of VR laboratories in chemistry education was initially limited and research-driven, in recent years, there has been a rapid expansion of interest, particularly with the increased accessibility of head-mounted display systems. Multiple studies have shown that integrating VR into chemistry laboratory instruction improves student engagement, conceptual understanding, and contextualization of abstract concepts.<sup>33,34</sup> Fundamental topics such as atomic structure, chemical bonding, molecular geometry, and reactivity are often challenging to convey using traditional teaching approaches, as they lie beyond direct sensory experience. Immersive VR and augmented reality (AR) frameworks, particularly when combined with haptic or interactive elements, enable more intuitive learning by allowing students to visualize and interact with chemical phenomena in three dimensions.<sup>35,36</sup> VR is generally more effective than passive instructional methods and can serve as an effective complementary tool alongside hands-on laboratory activities.<sup>24</sup>

At secondary and tertiary educational levels, immersive and augmented VR technologies, including three-dimensional user interfaces and head-mounted displays, have been successfully employed to support the visualization of intermolecular interactions, chemical bonding, and molecular structure.<sup>37</sup> Recent studies further demonstrate that VR/AR integration enhances student motivation, competence development, communication skills, and

self-directed learning when compared to traditional instructional approaches.<sup>38</sup> VR has been implemented in advanced inorganic chemistry courses to facilitate understanding of coordination chemistry and molecular orbital theory, particularly for upper-level undergraduate students.<sup>39</sup> Remote and collaborative VR-based laboratory activities have also been explored for experiments such as flame-color tests, metal-ion separation, and qualitative analysis, with assessment results indicating effective learning outcomes and improved collaboration.<sup>40,41</sup>

Maintaining a safe learning environment is a critical consideration in chemistry education, particularly when introducing students with limited laboratory experience to experimental work. Integrating VR with traditional instruction reinforces theoretical knowledge through immersive demonstrations, thereby supporting students' understanding of complex concepts before physical laboratory engagement.<sup>42</sup> Systems such as ChemistryVR and other VR-based laboratory simulations have therefore been proposed as practical solutions to common challenges in traditional laboratory instruction, particularly for novice learners.<sup>43</sup> VR has been successfully employed in biochemistry and molecular science courses, including large-scale implementations involving hundreds of undergraduate students, offering low-cost, portable, and less hazardous alternatives to conventional laboratory settings.<sup>44</sup> Game-based learning using The virtual Chemistry classroom for chemical Bonding (VC3B) has been implemented in middle-school chemistry classes to gauge its influence on students' understanding of chemical bonding formulas, which was assessed using a paper-based test, ratings of performance by expert teachers, statistical analysis using ANOVA and SPSS v23 and a satisfaction survey questionnaire, where students were divided randomly into 3 different study groups including textbooks, online and VC3B group. The VC3B group was found to be more interactive and efficient than traditional teaching methods, achieving an 81.51% success rate, compared with the conventional textbook group at 60.6% and the online lectures at 66.36%.<sup>45</sup> VR interaction techniques using the Oculus Quest V.1 device have been reported to influence students' engagement in a study that divided participants into 3 groups: text-based, VR with hand gestures, and VR with ray-casting. The ray-casting interaction technique was more interactive, practical, and accurate, resulting in faster task completion and better learning outcomes for STEM students.<sup>46</sup>

Beyond education, the broader digitalization of chemistry through artificial intelligence, VR, and metaverse frameworks is increasingly supporting research in catalyst design, molecular modeling, and reaction pathway optimization.<sup>23,47</sup> Interactive molecular dynamics in VR (iMD-VR), for example, has been shown to produce measurable learning gains and strong motivational effects in undergraduate organic chemistry courses.<sup>48</sup> Nevertheless, despite the numerous advantages of VR-based instruction, including enhanced visualization, safety, cost efficiency, and engagement, certain aspects of laboratory practice, such as routine cleanup behaviors and fine motor skills, are less effectively replicated in virtual environments.<sup>49,50</sup> These observations underscore the importance of hybrid instructional models that combine immersive VR with hands-on laboratory experience.



From a financial perspective, the hybrid VR model is scalable, as a single recorded module can be reused across multiple cohorts without additional cost. Standalone VR headsets are now relatively affordable (typically ~\$300–\$500 in 2026), significantly lower than traditional laboratory infrastructure costs. Furthermore, the recorded VR modules in published studies can be readily adapted into high-quality first-person 2D instructional videos when VR access is limited, thereby enhancing accessibility without additional costs.

### Case study teaching model

The hybrid laboratory session was developed following analysis of student feedback collected across multiple undergraduate courses and student backgrounds at Khalifa University of Science and Technology, United Arab Emirates. A survey involving approximately 109 students from biomedical engineering, chemistry, chemical engineering, mechanical engineering, cell and molecular biology and electrical engineering majors indicated a preference for incorporating VR into laboratory teaching modules (Fig. 1). These findings motivated the implementation of a VR-assisted laboratory session within an advanced inorganic chemistry undergraduate course designed for third- or fourth-year BSc chemistry students. 15 students participated throughout the session. Rather than serving as a comparative educational study, this work focuses on demonstrating the design, implementation, and feasibility of a hybrid instructional framework that integrates VR with hands-on experimentation for sustainable synthesis. The case study directly translates the outlined sustainability and educational motivations into practical teaching practice and builds upon the literature-based overview of VR applications in chemistry education.

The hybrid laboratory session was designed to achieve the following learning objectives:

1. Enhance students' understanding of green chemistry principles, catalysis and sustainability within modern laboratory practice.



Fig. 1 Survey of 109 students on the preference of incorporating VR into laboratory teaching modules.

2. Introduce the principles of mechanochemical synthesis and the evaluation of green chemistry metrics.
3. Integrate inorganic and organic chemistry concepts within an advanced, multistep laboratory workflow.
4. Design, synthesize and characterize Cu–NHC complex using sustainable methodologies.

The VR activities supported procedural accuracy, safety awareness, and conceptual understanding. At the same time, mechanochemistry provided a tangible example of sustainable chemical technology in practice and aligned the session with the United Nations Sustainable Development Goals (SDG 4: Quality Education and SDG 12: Responsible Consumption and Production).

VR-based laboratory orientation reduces procedural uncertainty and mitigates safety risks. By combining solvent-free mechanochemistry with immersive visualization, the session minimizes the laboratory time demands of a 60-minute synthesis while reducing exposure to hazardous materials, without compromising educational depth. Mechanochemistry provides a pedagogically rich context, as solid-state reactions challenge students to think beyond traditional solution-phase paradigms and emphasize concepts such as energy transfer, reagent proximity, and solubility-independent reactivity.<sup>5</sup>

Copper–NHC complexes of the general formula  $[\text{Cu}(\text{X})(\text{NHC})]$  ( $\text{X}$  = halide) play an essential role in contemporary medicinal chemistry applications and catalysis, including cross-coupling reactions, redox processes, and C–C bond formation.<sup>8</sup> Their reactivity is closely associated with the strong  $\sigma$ -donating character of NHC ligands and their ability to stabilize reactive copper centers. From a teaching perspective, the ability of Cu–NHC complexes to operate under aerobic conditions provides a valuable contrast to conventional inert-atmosphere protocols and reinforces key green chemistry concepts. The utilized mechanochemical route is based on an established mechanochemical strategy for Cu–NHC synthesis, translating these advances into a simple synthesis approach and pedagogically accessible laboratory format.<sup>18</sup> Fig. 2

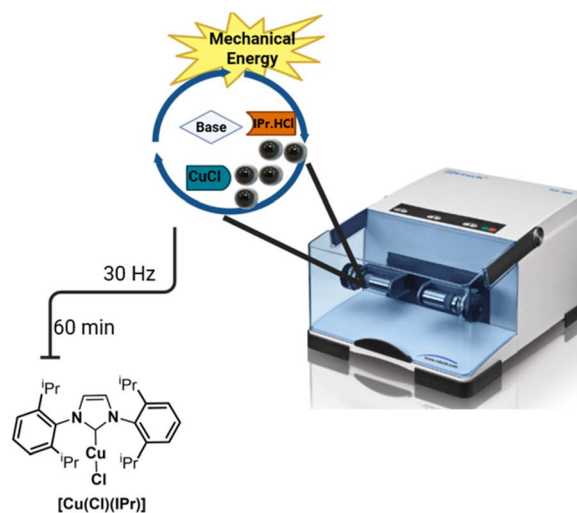


Fig. 2 Mechanochemical reactions in the teaching model.<sup>18</sup>



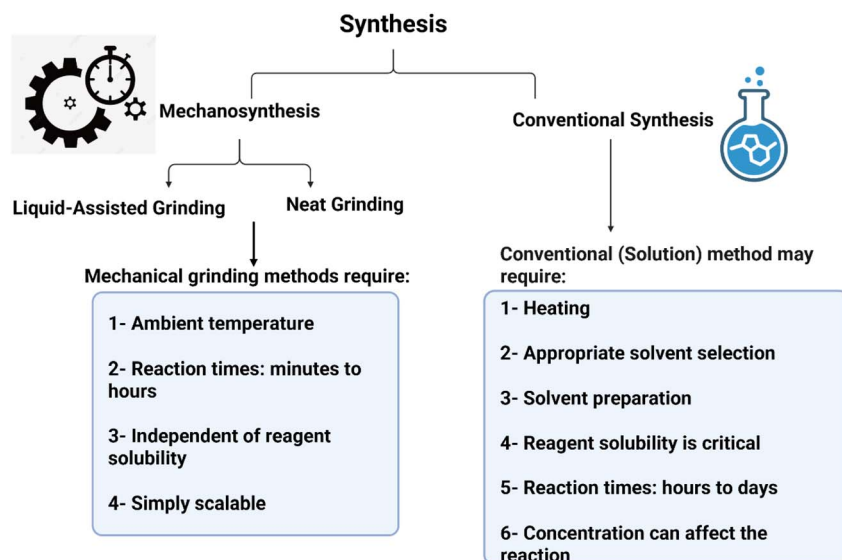


Fig. 3 Demonstration of the introduction to synthetic methods.

illustrates the mechanochemical reaction scheme used in the teaching materials, while Fig. 3 presents an example of mechanochemistry-focused instructional content adapted from lecture slides and posters.

The complete workflow of the hybrid session is summarized in Fig. 4, and representative screenshots from the VR modules and sample immersive videos are provided in the SI.

The session was structured as a single, integrated in-lab activity that combined virtual and physical components in

real time. Students engaged with VR-based instructional modules during the laboratory session to introduce laboratory safety guidelines, reaction preparation, and the mechanochemical reaction. The VR resources (including immersive videos) are provided in the SI, and Fig. 5 presents screenshots from these videos.

The hands-on components of the session included preparing and launching the mechanochemical ball-milling reaction, performing the reaction work-up and isolating the product.

Phase	Description	Time
<b>Pre-Lab</b>	Pre-lab questions	5 min
<b>Safety &amp; Orientation</b>	Safety overview, learning objectives, and VR introduction	10 min
<b>Mechanochemical Background</b>	Introduction to mechanochemistry and synthesis comparison	10 min
<b>VR Module 1</b>	Virtual reaction preparation	3 min
<b>Hands-On Lab 1</b>	Students prepare the reaction mixture	5 min
<b>VR Module 2</b>	Ball-milling visualization of copper NHC synthesis	5 min activity
<b>Hands-On Lab 2</b>	Launch the milling process	5 min
<b>VR Module 3</b>	Virtual work-up demonstration	3–4 min
<b>Hands-On Lab 3</b>	Work-up, filtration, evaporation, precipitation, and drying of the previous sample by students	60 min + 5 min activity
<b>VR Module 4</b>	NMR demonstration, interpretation, and Q&A	25 min
<b>Wrap-Up Discussion</b>	Yields, NMR interpretation, green chemistry reflection, and lab report discussion	20 min

Fig. 4 Outline of the hybrid laboratory session.



## 1. Reaction Preparation



## 3-Work-Up and Product isolation



## 2. Mechanochemical Synthesis



## 4-NMR Characterization



Fig. 5 Screenshot examples of VR videos.

While students initiated the ball-milling process, they did not wait for its full duration; instead, students proceeded with the work-up and purification steps using reaction mixtures prepared in advance by the instructor or previous cohorts. The VR visualization condensed the synthesis step, which typically takes approximately 60 min under real laboratory conditions, into a brief, immersive representation, allowing students to contextualize key stages while concurrently working on other experimental steps. This approach avoids additional waste, as student-initiated samples are retained and used by subsequent cohorts, ensuring continuity of the workflow. The student-prepared ball-milled mixtures were retained for use in subsequent sessions. This integrated workflow ensured efficient use of laboratory time while maintaining student engagement with all key experimental stages from reaction preparation and mechanical grinding to product isolation and purification.

Restricted access to advanced analytical instrumentation, particularly NMR spectroscopy, remains a standard limitation in UG teaching chemistry laboratories. While NMR is essential for structural characterization, direct student access is often constrained by safety considerations, instrument availability, and curricular time limitations. In this session, the final stage involved VR-guided visualization of the characterization of the purified Cu-NHC complex, focusing on NMR instrument operation, data acquisition and spectral interpretation. This approach reinforced the connection between synthesis and characterization without extending laboratory time or introducing additional constraints. To ensure broad transferability, the VR-based NMR modules were complemented by high-quality immersive videos, enabling adoption of the same teaching framework at institutions without immersive VR infrastructure.

Student performance was evaluated based on the correct handling, purification, and isolation of the target Cu-NHC

complex within the allocated laboratory time, as well as the assessment of submitted laboratory reports. Students demonstrated improved preparedness for hands-on experimentation, enhanced understanding of mechanochemical synthesis and green chemistry principles, and increased familiarity with the workflow and interpretation of NMR spectroscopy. Students completed written questions and a poster on laboratory concepts and calculated green chemistry metrics (*e.g.*, atom economy, environmental factor, and mass intensity). A representative student poster summarizing the experiment is presented as Fig. 6, while the complete lab manual and student report are provided in the SI.

#### Limitation of the study

Conventional 2D lab recordings were previously used as a baseline instructional method, with student reports confirming successful procedural understanding and analysis. However, a direct controlled comparison with the VR format was not conducted in this study. Notably, the VR recordings can also function as high-quality first-person instructional videos when VR platforms are not available, and future work will include controlled comparisons to quantitatively evaluate the added value of immersion.

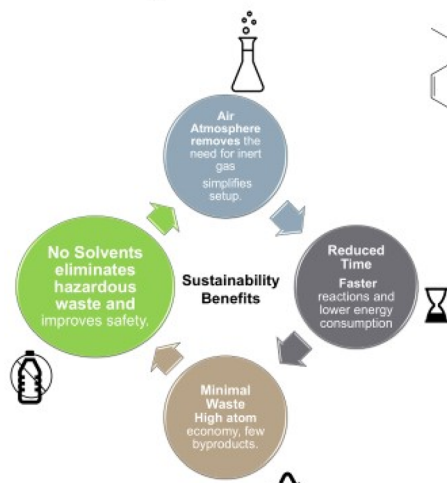
## Experimental part

All procedures involving human participants were conducted in accordance with UAE guidelines and Khalifa University institutional guidelines. The study protocol, "Exploring the Impact of Virtual Reality Simulation Labs on Undergraduate Science Students' Perception of Complex Scientific Concepts" (Protocol No. H25-026), was reviewed and approved by the Research Ethics Committee (REC) of Khalifa University of Science and Technology. Written informed consent was obtained from all



# Mechanosynthesis of [Cu(Cl)(NHC)] under Aerobic Conditions: Hybrid Teaching Lab

## Sustainability Benefits



### Mechanochemical Synthesis:

- Solvent-free
- Rapid ( $\approx 60$  min)
- Low energy demand

### Traditional Synthesis:

- High solvent use
- Long reaction times
- High energy consumption

## Key VR Session Benefits

- VR session clarified the experimental procedure sequence before hands-on work
- 3D VR visualization increased confidence and understanding of safe lab practices
- VR videos clearly explained key steps: milling, product isolation, and NMR characterization
- VR content closely matched the physical lab experiment, bridging theory and practice
- VR reduced risks associated with safety and chemical handling prior to lab work

## Mechanochemistry Process



## Green Metrics and calculations

$$\text{Atom economy (AE)} = \frac{\text{MW of the desired product}}{\text{MW weight of all reactant}} \times 100\% = \frac{487}{425.04+98.99} \times 100\% = 92.90\%$$

$$\text{Reaction Mass Efficiency (RME)} = \frac{\text{mass of product}}{\text{total mass of reactants}} \times 100\% = \frac{255}{443.0} \times 100\% = 57.56\%$$

$$\text{Mass Intensity (MI)} = \frac{\text{Total mass of all material used}}{\text{Mass of the product}} = \frac{443.0}{255} = 1.74$$

$$\text{Optimum Efficiency (OE)} = \frac{\text{RME}}{\text{AE}} \times 100\% = \frac{57.56}{92.9} \times 100\% = 62.95\%$$

$$\text{Environmental Factor (E-factor)} = \text{MI} - 1 = 0.74$$

## Conclusion & Recommendations

- VR labs mitigate safety risks, expand accessibility, and support diverse learners
- Future improvements: adaptive protocols, real-time green metrics calculator, collaborative virtual laboratory spaces.



Fig. 6 Representative student poster created following completion of the experiment, reflecting key learning outcomes and takeaways.

participants prior to participation in the study. Participation was voluntary; survey and MCQ responses were collected anonymously, participants were free to withdraw at any time without penalty, and participants were advised to discontinue the VR activity if they experienced dizziness or discomfort.

Structured procedures for students are provided in the SI lab manual.

## Mechanosynthesis of [Cu(Cl)(IPr)] under aerobic conditions

A stainless-steel milling jar (10 mL) equipped with five stainless-steel balls (7 mm diameter) was charged with 1,3-bis(2,6-disisopropylphenyl)imidazolium chloride IPr.HCl (200.0 mg, 0.473 mmol, 1.0 equiv), CuCl (47.0 mg, 0.473 mmol, 1.0 equiv.), and K<sub>2</sub>CO<sub>3</sub> (196.0 mg, 1.420 mmol, 3.0 equiv.). The jar was sealed, placed in a vibrational ball mill, and subjected to 2 cycles (30 min each) at 25 rpm. The crude product was extracted with acetone (15 mL) and filtered through silica gel (SiO<sub>2</sub>). The solvent volume was reduced under vacuum to approximately 7–8 mL, allowing the product to precipitate upon the addition of pentane (10 mL) as a cosolvent and cooling the solution. The [Cu(Cl)(IPr)] product was filtered, yielding 66% (152 mg). Melting point: 311 ± 2 °C.

The reaction can be performed in a single continuous run; however, it was divided into two 30-minute intervals with a ~2 minute rest period to limit thermal buildup and protect frequently used equipment, as mechanochemical milling is known to generate localized heating.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.49 (t, 3J = 7.5 Hz, 2H, ArH), 7.30 (d, 3J = 7.5 Hz, 4H, ArH), 7.14 (s, 2H, NCH=CHN), 2.59–2.53 (m, 4H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.29 (d, 3J = 7 Hz, 12H, CH–CH<sub>3</sub>), 1.23 (d, 3J = 7 Hz, 12H, CH–CH<sub>3</sub>). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  = 145.58, 134.38, 130.60, 124.23, 123.14, 28.75, 24.85, 23.89. The reaction can also be performed on a scale of 75.0 mg of IPr.HCl. Yield = 65%.

## Conclusion

This work demonstrates the successful design and implementation of a hybrid teaching model that integrates VR-assisted instruction with sustainable mechanochemical synthesis in an advanced undergraduate inorganic chemistry laboratory, informed by positive feedback from a survey of 109 students favoring the integration of VR in lab sessions. By combining solvent-free mechanochemical synthesis of a Cu–NHC



complex with immersive VR visualization, the module provides a pedagogically practical framework that enhances laboratory preparedness, procedural understanding, and safety awareness while preserving essential hands-on experimental skills. The use of mechanochemistry as the synthetic platform aligns naturally with green chemistry principles and the United Nations Sustainable Development Goals, offering students direct exposure to contemporary, environmentally responsible chemical practices. The VR-assisted components of the laboratory session enabled students to visualize complex experimental workflows, including reaction setup, ball milling, purification, and NMR characterization, before physical execution. This pre-laboratory immersion reduced procedural uncertainty and optimized laboratory time without replacing tactile laboratory experience. Notably, the hybrid approach addresses well-documented limitations of both traditional laboratory instruction and fully virtual laboratories by leveraging the strengths of each: immersive visualization and safety in VR, combined with experiential learning through physical experimentation.

Rather than serving as a comparative educational assessment, this study focuses on the feasibility, scalability, and transferability of a hybrid VR-mechanochemistry teaching framework. The instructional design was informed by student feedback and supported by reusable two- and three-dimensional digital resources, enabling adoption across institutions with varying levels of laboratory infrastructure and access to VR technology. The inclusion of VR-guided analytical characterization further extends the module's educational reach, particularly in contexts where undergraduate access to advanced instrumentation, such as NMR spectroscopy, is limited. Overall, this case study illustrates how emerging digital technologies can be meaningfully integrated into undergraduate laboratory curricula to support sustainable synthesis, enhance student engagement, and modernize chemical education. The hybrid teaching model presented here offers a practical pathway for incorporating green chemistry, mechanochemistry, and immersive visualization into advanced laboratory instruction and provides a foundation for future expansion into other areas of inorganic, organometallic, and materials chemistry education. Future work will focus on implementing the hybrid VR framework in a broader range of courses and on an elaborate analysis of the institutional survey results.

## Ethical statement

This study involving human participants was reviewed and approved by the Research Ethics Committee of Khalifa University of Science and Technology (Approval No. H25-026).

## Author contributions

Abeer Shunnar and Abdulrahman Aoudi contributed to investigation, methodology, and writing of the original draft. Suleiman Musa contributed to investigation and writing – review and editing. Mohamed Aslam and Safaa Mohamad Al Yousif

contributed to supervision and validation. Aya Shanti and Gihan Daw El Bait contributed to data curation and formal analysis. Amin Ahmed Babiker Ali contributed to conceptualization, resources, and writing – review and editing. Meriem Bildsten contributed to resources, investigation, and writing – review and editing. Emilia Oueis and Andrew B. Lowe contributed to project administration, conceptualization, and writing – review and editing. Janah Shaya contributed to conceptualization, resources, investigation, methodology, and writing – review and editing.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

The data supporting this study, including instructional resources, anonymized survey materials, NMR spectra, and representative student outputs, are available in the manuscript and in the supplementary information (SI) accompanying this article. Supplementary information is available. See DOI: <https://doi.org/10.1039/d6su00054a>.

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## References

- 1 P. Anastas and N. Eghbali, Green Chemistry: Principles and Practice, *Chem. Soc. Rev.*, 2010, **39**(1), 301–312.
- 2 United Nations Development Programme. What are the Sustainable Development Goals? <https://www.undp.org/sustainable-development-goals>.
- 3 P. J. Dunn, The Importance of Green Chemistry in Process Research and Development, *Chem. Soc. Rev.*, 2012, **41**(4), 1452–1461, DOI: [10.1039/c1cs15041c](https://doi.org/10.1039/c1cs15041c).
- 4 S. L. James, C. J. Adams, C. Bolm, D. Braga, P. Collier, T. Friščić, F. Grepioni, K. D. M. Harris, G. Hyett, W. Jones, A. Krebs, J. Mack, L. Maini, A. G. Orpen, I. P. Parkin, W. C. Shearouse, J. W. Steed and D. C. Waddell, Mechanochemistry: Opportunities for New and Cleaner Synthesis, *Chem. Soc. Rev.*, 2012, **41**, 413–447, DOI: [10.1039/c1cs15171a](https://doi.org/10.1039/c1cs15171a).



- 5 T. Friščić, C. Mottillo and H. M. Titi, Mechanochemistry for Synthesis, *Angew. Chem.*, 2020, **132**(3), 1030–1041, DOI: [10.1002/ange.201906755](https://doi.org/10.1002/ange.201906755).
- 6 F. Quintin, J. Pinaud, F. Lamaty and X. Bantreil, Mechanochemistry of Noels-Type NHC-Ruthenium Complexes and Applications in Ring-Opening Metathesis Polymerization, *Organometallics*, 2020, **39**(5), 636–639, DOI: [10.1021/acs.organomet.0c00013](https://doi.org/10.1021/acs.organomet.0c00013).
- 7 F. T. Gomollón-Bel, Chemical Innovations That Will Change Our World, *Chem. Int.*, 2020, **42**(4), 3–9, DOI: [10.1515/ci-2020-0402](https://doi.org/10.1515/ci-2020-0402).
- 8 J. D. Egbert, C. S. J. Cazin and S. P. Nolan, Copper N-Heterocyclic Carbene Complexes in Catalysis, *Catal. Sci. Technol.*, 2013, **3**(4), 912–926, DOI: [10.1039/c2cy20816d](https://doi.org/10.1039/c2cy20816d).
- 9 J. Haneef and S. Ali, Medicinal Mechanochemistry: Sustainable and Efficient Route towards Synthesis of Active Pharmaceutical Ingredients, *Sustain. Chem. Pharm.*, 2025, **45**, 102044, DOI: [10.1016/j.scp.2025.102044](https://doi.org/10.1016/j.scp.2025.102044).
- 10 M. Hachem, SARS-CoV-2 Journey to the Brain with a Focus on Potential Role of Docosahexaenoic Acid Bioactive Lipid Mediators, *Biochimie*, 2021, **184**, 95–103, DOI: [10.1016/j.biochi.2021.02.012](https://doi.org/10.1016/j.biochi.2021.02.012).
- 11 M. Lagarde, M. Hachem, M. Picq, M. Guichardant and N. Bernoud-Hubac, AceDoPC, a Structured Phospholipid to Target the Brain with Docosahexaenoic Acid, *OCL:Oilseeds Fats, Crops Lipids*, 2016, **23**(1), D102, DOI: [10.1051/ocl/2015061](https://doi.org/10.1051/ocl/2015061).
- 12 D. V. Aleksanyan and V. A. Kozlov, Mechanochemical Tools in the Synthesis of Organometallic Compounds, *Mendeleev Commun.*, 2023, **33**(3), 287–301, DOI: [10.1016/j.mencom.2023.04.001](https://doi.org/10.1016/j.mencom.2023.04.001).
- 13 J. Sherwood, J. H. Clark, I. J. S. Fairlamb and J. M. Slattery, Solvent Effects in Palladium Catalysed Cross-Coupling Reactions, *Green Chem.*, 2019, **21**(9), 2164–2213, DOI: [10.1039/c9gc00617f](https://doi.org/10.1039/c9gc00617f).
- 14 J. El-Maiss, T. M. El Dine, C. S. Lu, I. Karamé, A. Kanj, K. Polychronopoulou and J. Shaya, Recent Advances in Metal-Catalyzed Alkyl-Boron (C(Sp<sup>3</sup>))–c(Sp<sup>2</sup>)) Suzuki-Miyaura Cross-Couplings, *Catalysts*, 2020, **10**(3), 296, DOI: [10.3390/catal10030296](https://doi.org/10.3390/catal10030296).
- 15 R. S. Rao, M. Bashri, M. I. H. Mohideen, I. Yildiz, D. Shetty and J. Shaya, Recent Advances in Heterogeneous Porous Metal–Organic Framework Catalysis for Suzuki-Miyaura Cross-Couplings, *Heliyon*, 2024, **10**(23), e40571, DOI: [10.1016/j.heliyon.2024.e40571](https://doi.org/10.1016/j.heliyon.2024.e40571).
- 16 K. Kubota and H. Ito, Mechanochemical Cross-Coupling Reactions, *Trends Chem.*, 2020, **2**(12), 1066–1081, DOI: [10.1016/j.trechm.2020.09.006](https://doi.org/10.1016/j.trechm.2020.09.006).
- 17 M. Marinelli, C. Santini and M. Pellei, Recent Advances in Medicinal Applications of Coinage-Metal (Cu and Ag) N-Heterocyclic Carbene Complexes, *Curr. Top. Med. Chem.*, 2016, **16**(26), 2995–3017, DOI: [10.2174/1568026616666160506145408](https://doi.org/10.2174/1568026616666160506145408).
- 18 A. Shunnar, R. S. Rao, M. Aslam, S. Stephen, H. Al Saraiher, A. B. Lowe and J. Shaya, Mechanochemistry in Senior Undergraduate Laboratory: NHC Complexes, Catalysis, and Sonogashira Cross-Coupling, *J. Chem. Educ.*, 2025, **102**(7), 2887–2895, DOI: [10.1021/acs.jchemed.4c01259](https://doi.org/10.1021/acs.jchemed.4c01259).
- 19 P. Bellotti, M. Koy, M. N. Hopkinson and F. Glorius, Recent Advances in the Chemistry and Applications of N-Heterocyclic Carbenes, *Nat. Rev. Chem.*, 2021, **5**(10), 711–725, DOI: [10.1038/s41570-021-00321-1](https://doi.org/10.1038/s41570-021-00321-1).
- 20 F. Lazreg, F. Nahra and C. S. J. Cazin, Copper-NHC Complexes in Catalysis, *Coord. Chem. Rev.*, 2015, **293–294**, 48–79, DOI: [10.1016/j.ccr.2014.12.019](https://doi.org/10.1016/j.ccr.2014.12.019).
- 21 F. Bru, S. M. P. Vanden Broeck, G. Pisanò, K. De Buysser and C. S. J. Cazin, Learning Green Chemistry Principles by Comparing Three Synthetic Routes to a Copper-NHC (NHC = N-Heterocyclic Carbene) Complex, *J. Chem. Educ.*, 2023, **100**(6), 2359–2366, DOI: [10.1021/acs.jchemed.2c01134](https://doi.org/10.1021/acs.jchemed.2c01134).
- 22 R. S. Mohan and M. P. Mejia, Environmentally Friendly Organic Chemistry Laboratory Experiments for the Undergraduate Curriculum: A Literature Survey and Assessment, *J. Chem. Educ.*, 2020, **97**(4), 943–959, DOI: [10.1021/acs.jchemed.9b00753](https://doi.org/10.1021/acs.jchemed.9b00753).
- 23 X. Zhu, Toward the Uniform of Chemical Theory, Simulation, and Experiments in Metaverse Technology, *Precis. Chem.*, 2023, **1**(4), 192–198, DOI: [10.1021/prechem.3c00045](https://doi.org/10.1021/prechem.3c00045).
- 24 P. Chan, T. Van Gerven, J. L. Dubois and K. Bernaerts, Virtual Chemical Laboratories: A Systematic Literature Review of Research, Technologies and Instructional Design, *Comput. Educ. Open*, 2021, **2**, 100053, DOI: [10.1016/j.caeo.2021.100053](https://doi.org/10.1016/j.caeo.2021.100053).
- 25 K. Altmeyer, S. Kapp, M. Thees, S. Malone, J. Kuhn and R. Brünken, The Use of Augmented Reality to Foster Conceptual Knowledge Acquisition in STEM Laboratory Courses—Theoretical Background and Empirical Results, *Br. J. Educ. Technol.*, 2020, **51**(3), 611–628, DOI: [10.1111/bjet.12900](https://doi.org/10.1111/bjet.12900).
- 26 A. Riganelli, O. Gervasi, A. Laganà and M. Alberti, A Multiscale Virtual Reality Approach to Chemical Experiments, *Lect. Notes Comput. Sci.*, 2003, **2658**, 324–330, DOI: [10.1007/3-540-44862-4\\_35](https://doi.org/10.1007/3-540-44862-4_35).
- 27 M. Limniou, D. Roberts and N. Papadopoulos, Full Immersive Virtual Environment CAVETM in Chemistry Education, *Comput. Educ.*, 2008, **51**(2), 584–593, DOI: [10.1016/j.compedu.2007.06.014](https://doi.org/10.1016/j.compedu.2007.06.014).
- 28 A. S. Lang and J. C. Bradley, Chemistry in Second Life, *Chem. Cent. J.*, 2009, **3**(1), 1–20, DOI: [10.1186/1752-153X-3-14](https://doi.org/10.1186/1752-153X-3-14).
- 29 J. Georgiou, K. Dimitropoulos and a. A. Manitsaris, Virtual Reality Laboratory for Distance Education in Chemistry, *World Acad. Sci. Eng. Technol.*, 2007, **1**(11), 345–352.
- 30 M. O'Connor, H. M. Deeks, E. Dawn, O. Metatla, A. Roudaut, M. Sutton, L. M. Thomas, B. R. Glowacki, R. Sage, P. Tew, M. Wonnacott, P. Bates, A. J. Mulholland and D. R. Glowacki, Sampling Molecular Conformations and Dynamics in a Multiuser Virtual Reality Framework, *Sci. Adv.*, 2018, **4**(6), 1–9, DOI: [10.1126/sciadv.aat2731](https://doi.org/10.1126/sciadv.aat2731).
- 31 K. Winkelmann, W. Keeney-Kennicutt, D. Fowler and M. D. Macik, Implementation, and Assessment of General Chemistry Lab Experiments Performed in the Virtual



- World of Second Life, *J. Chem. Educ.*, 2017, **94**(7), 849–858, DOI: [10.1021/acs.jchemed.6b00733](https://doi.org/10.1021/acs.jchemed.6b00733).
- 32 K. Winkelmann, W. Keeney-Kennicutt, D. Fowler, M. Lazo Macik, P. Perez Guarda and C. Joan Ahlborn, Learning Gains and Attitudes of Students Performing Chemistry Experiments in an Immersive Virtual World, *Interact. Learn. Environ.*, 2020, **28**(5), 620–634, DOI: [10.1080/10494820.2019.1696844](https://doi.org/10.1080/10494820.2019.1696844).
- 33 A. Rizvan, A. Luiza and Y. Anna, Enhancing Chemistry Education's Relevance and Comprehension through Immersive Virtual Reality, *E3S Web Conf.*, 2023, **451**, 06013, DOI: [10.1051/e3sconf/202345106013](https://doi.org/10.1051/e3sconf/202345106013).
- 34 T. L. Lai, Y. S. Lin, C. Y. Chou and H. P. Yueh, Evaluation of an Inquiry-Based Virtual Lab for Junior High School Science Classes, *J. Educ. Comput. Res.*, 2022, **59**(8), 1579–1600, DOI: [10.1177/07356331211001579](https://doi.org/10.1177/07356331211001579).
- 35 T. Weymuth and M. Reiher, Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry, *Chimia*, 2021, **75**(2), 45–49, DOI: [10.2533/chimia.2021.45](https://doi.org/10.2533/chimia.2021.45).
- 36 A. Fombona-Pascual, J. Fombona and E. Vázquez-Cano, VR in Chemistry, a Review of Scientific Research on Advanced Atomic/Molecular Visualization, *Chem. Educ. Res. Pract.*, 2022, **23**(2), 300–312, DOI: [10.1039/d1rp00317h](https://doi.org/10.1039/d1rp00317h).
- 37 Z. A. Jiménez, Teaching and Learning Chemistry via Augmented and Immersive Virtual Reality, *ACS Symp. Ser.*, 2019, **1318**, 31–52, DOI: [10.1021/bk-2019-1318.ch003](https://doi.org/10.1021/bk-2019-1318.ch003).
- 38 E. Amirbekova, N. Shertayeva and E. Mironova, Teaching Chemistry in the Metaverse: The Effectiveness of Using Virtual and Augmented Reality for Visualization, *Front. Educ.*, 2023, **8**(January), 1–9, DOI: [10.3389/feeduc.2023.1184768](https://doi.org/10.3389/feeduc.2023.1184768).
- 39 R. Dai, J. A. Laureanti, M. Kopelevich and P. L. Diaconescu, Developing a Virtual Reality Approach toward a Better Understanding of Coordination Chemistry and Molecular Orbitals, *J. Chem. Educ.*, 2020, **97**(10), 3647–3651, DOI: [10.1021/acs.jchemed.0c00469](https://doi.org/10.1021/acs.jchemed.0c00469).
- 40 H. Fujiwara, T. Kano and T. Akakura, Development of Collaborative Chemistry Experiment Environment Using VR, *Lect. Notes Comput. Sci.*, 2021, **12766**(LNCS), 14–26, DOI: [10.1007/978-3-030-78361-7\\_2](https://doi.org/10.1007/978-3-030-78361-7_2).
- 41 Z. Naz, A. Azam, M. U. G. Khan, T. Saba, S. Al-Otaibi and A. Rehman, Development and Evaluation of Immersive VR Laboratories of Organic Chemistry and Physics for Students Education, *Phys. Scr.*, 2024, **99**(5), 056101, DOI: [10.1088/1402-4896/ad3024](https://doi.org/10.1088/1402-4896/ad3024).
- 42 N. Ali and S. Ullah, Review to Analyze and Compare Virtual Chemistry Laboratories for Their Use in Education, *J. Chem. Educ.*, 2020, **97**(10), 3563–3574, DOI: [10.1021/acs.jchemed.0c00185](https://doi.org/10.1021/acs.jchemed.0c00185).
- 43 G. Jiang, X. Xia, Y. Li, H. N. Liang, and P. Hui, ChemistryVR: Enhancing Educational Experiences through Virtual Chemistry Lab Simulations, *Proc. - SIGGRAPH Asia 2024 Educ. Forum, SA 2024*, 2024, No. December, DOI: [10.1145/3680533.3697068](https://doi.org/10.1145/3680533.3697068).
- 44 T. Qin, M. Cook and M. Courtney, Exploring Chemistry with Wireless, PC-Less Portable Virtual Reality Laboratories, *J. Chem. Educ.*, 2021, **98**(2), 521–529, DOI: [10.1021/acs.jchemed.0c00954](https://doi.org/10.1021/acs.jchemed.0c00954).
- 45 H. Rahman, S. A. Wahid, F. Ahmad and N. Ali, Game-Based Learning in Metaverse: Virtual Chemistry Classroom for Chemical Bonding for Remote Education, *Educ. Inf. Technol.*, 2024, **29**(15), 19595–19619, DOI: [10.1007/s10639-024-12575-5](https://doi.org/10.1007/s10639-024-12575-5).
- 46 S. Qorbani, S. Dalili, A. Arya and C. Joslin, Assessing Learning in an Immersive Virtual Reality: A Curriculum-Based Experiment in Chemistry Education, *Educ. Sci.*, 2024, **14**(5), 476, DOI: [10.3390/educsci14050476](https://doi.org/10.3390/educsci14050476).
- 47 S. N. Suzuki, H. Kanematsu, D. M. Barry, N. Ogawa, K. Yajima, K. T. Nakahira, T. Shirai, M. Kawaguchi, T. Kobayashi and M. Yoshitake, Virtual Experiments in Metaverse and Their Applications to Collaborative Projects: The Framework and Its Significance, *Procedia Comput. Sci.*, 2020, **176**, 2125–2132, DOI: [10.1016/j.procs.2020.09.249](https://doi.org/10.1016/j.procs.2020.09.249).
- 48 J. B. Ferrell, J. P. Campbell, D. R. McCarthy, K. T. McKay, M. Hensinger, R. Srinivasan, X. Zhao, A. Wurthmann, J. Li and S. T. Schneebeli, Chemical Exploration with Virtual Reality in Organic Teaching Laboratories, *J. Chem. Educ.*, 2019, **96**(9), 1961–1966, DOI: [10.1021/acs.jchemed.9b00036](https://doi.org/10.1021/acs.jchemed.9b00036).
- 49 E. Hu-Au and S. Okita, Exploring Differences in Student Learning and Behavior Between Real-Life and Virtual Reality Chemistry Laboratories, *J. Sci. Educ. Technol.*, 2021, **30**(6), 862–876, DOI: [10.1007/s10956-021-09925-0](https://doi.org/10.1007/s10956-021-09925-0).
- 50 R. M. Broyer, K. Miller, S. Ramachandran, S. Fu, K. Howell and S. Cutchin, Using Virtual Reality to Demonstrate Glove Hygiene in Introductory Chemistry Laboratories, *J. Chem. Educ.*, 2021, **98**(1), 224–229, DOI: [10.1021/acs.jchemed.0c00137](https://doi.org/10.1021/acs.jchemed.0c00137).

