School of Education

Evaluation of Students' Chemistry Learning and Experiences in Collaborative Immersive Virtual Reality

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Declaration

To the best of my knowledge and belief this thesis contains no material previously published by any other person except where due acknowledgment has been made.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Human Ethics The research presented and reported in this thesis was conducted in accordance with the National Health and Medical Research Council National Statement on Ethical Conduct in Human Research (2007) – updated March 2014. The proposed research study received human research ethics approval from the Curtin University Human Research Ethics Committee (EC00262), Approval Number #HRE2020-0081

Signature: ....

Date: ....

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Abstract

Immersive virtual reality (iVR), with its advanced 3D visualisation and interactivity, offers an engaging science learning experience. While commonly used pre- and post-multiple-choice assessments demonstrate iVR's positive impact on students' information recall skills, limited studies have explored iVR's support for deeper conceptual understanding. Existing research has predominantly highlighted user perspectives, emphasising iVR as an engaging activity. However, how students' perceptions relate to their interactions and learning outcomes within iVR environments remains unclear.

This study addressed the gap in understanding the benefit of iVR by evaluating students' conceptual changes, interactions, and perceptions during iVR-based learning activities and comparing them with activities involving magnetic models. Twenty pairs of first-year undergraduate students went through a series of activities with magnetic models and iVR to learn about hydrogen bonding and its role in forming snowflakes. The videos of students' interactions and interviews with their hand-drawn diagrams were analysed with multimodal cross-case analysis.

Students, particularly pairs with alternative prior understanding, used the magnetic models' tactile feedback to individually explore the attraction and repulsion between water molecules in forming hydrogen bonding. In contrast, students, especially pairs with high prior knowledge, collaboratively interacted with a lattice structure of water molecules to establish links between water molecules (microscopic) and snowflakes (macroscopic). Compared with magnetic models, students perceived their iVR experience as a more collaborative problem-solving activity that helped them appreciate more complex 3D spatial arrangements of molecular structures. By exploring alternative ways to evaluate students' learning and experiences, this study revealed the significant roles played by students' prior knowledge and group composition in shaping their unique learning experience and scientific understanding within collaborative iVR environments.

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Statement of Contribution to Co-Authored Published Paper

This thesis includes the content of the co-authored paper "Students' use of magnetic models to learn hydrogen bonding and the formation of snowflakes", published in the *Journal of Chemical Education* in 2023. The bibliographic details of the paper, including all authors, are:

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I, Dewi Ayu Kencana Ungu, as the primary author, undertook the leading role in data collection, analysis, and manuscript writing. The co-authors contributed to data analysis for inter-rater reliability, reviewed the manuscript, and/or supervised the research.

Dewi Ayu Kencana Ungu ....

I, as a co-author, endorse that this level of contribution indicated above by the candidate is appropriate.

Mihye Won ....

David F. Treagust ....

Mauro Mocerino ....

Henry Matovu ....

Chin-Chung Tsai ....

Roy Tasker ....

Chapter 1. Introduction

1.1 Personal Motivation for Conducting Research

Explorations of new technologies have always excited me. At first, the technologies were only about fun through playing games, but they soon started to help me learn. When my teachers first taught me how to read English in class, I already engaged in English as a farmer or astronaut through computer games I played at home (e.g., Magic School Bus in Haugland and Ruíz (2002)). I did not even realise that I was learning through technology at that time. Fast forward to my 20s, I decided to take a job at an educational technology company because my excitement about technology in my early days was still in me.

My job at the educational technology company was to write a storyline for a virtual laboratory simulation. The goal of the simulation was to engage students in a mission to solve a problem using scientific approaches. For example, to help students learn about DNA, I put students in the shoes of forensic laboratory technicians who must identify a culprit based on a blood sample. The application targeted high school and university students, especially those with limited access to sophisticated laboratories. Students accessed our virtual laboratory simulation using their laptop or desktop computer, and their response fell along the lines of "This is such a fun way to learn!". It felt fantastic to hear such comments from students. I was getting better at developing educational content for the virtual laboratory until the Oculus Rift virtual reality headset was launched in 2016.

Immersive virtual reality (iVR) headset, such as Oculus Rift CV1 or S, completely blocks the view of the real world and allows the user to have a 360-degree view of a 3D virtual world (Angelov et al., 2020). The immersive experience offered by the iVR headset amazed everyone in our office, especially me. Like many companies at that time, we quickly adopted iVR for our virtual laboratories. Our approach was to convert all the content immediately so it could be displayed on both desktop and iVR. Students could now access the virtual laboratory using iVR headsets such as Google Daydream or Samsung Gear VR. The immediate responses from the teachers and students related to the new immersive experience increased students' motivation to learn. But the novelty effect did not last long. More teachers chose the desktop version because it was cheaper and had the same content as the VR version. So, I thought, what was the point of our effort to use iVR headsets for our virtual laboratory simulation?

My intention in embarking on this research is to better understand how students experience iVR for learning science. Science topics, including chemistry, are close to my heart because of my science background and years of making virtual science laboratory content. I also experienced the benefit of having a better understanding of science when I used technology in addition to a textbook. I also noticed that some educators were optimistic, while some were pessimistic about the potential of iVR for science learning (Bower et al., 2020; Lege & Bonner, 2020). However, this phenomenon was similar to what happened in the early 80s-90s when desktop computers were started to be used for learning (Pepi & Scheurman, 1996). With years of research in computer-supported learning, we now better understand how students use computers – it is different from interacting with the content from a textbook (Kozma, 1991; Mellon, 1999). My research is designed to explore the educational possibilities and limitations of iVR and inform educators about how students use and perceive iVR to learn scientific concepts. I will compare student learning in an iVR environment with students using magnetic models.

1.2 Rationale for Research

Immersive virtual reality (iVR) has unique visualisation and interactivity features. Unlike other media, iVR fully transports the user into a computer-generated world (Slater & Sanchez-Vives, 2016). The sense of being in the virtual world is induced by what the students can see and do with the aid of a head-mounted-display (HMD) headset or iVR headset (Cummings & Bailenson, 2016). When users (students) wear iVR headsets, the real space is no longer visible. Everywhere they looked, they could only see a 3D virtual world. The iVR system also tracks students' positions and body movements as input, allowing them to interact with the 3D virtual world by turning their heads or waving their hands. With its immersive 3D visualisation and intuitive interactivity, many educational researchers saw iVR as a learning media that could help students learn (Radianti et al., 2020).

Previous educational iVR studies explored the educational benefit of iVR by evaluating students before and after the activity. Multiple choice, fill-in-blank, or short answer questions were often used as pre- and post-tests to measure students' learning outcomes. For example, Liu et al. (2020) used multiple-choice questions to show that students who experienced iVR performed better in science than students who learned through traditional teaching methods.

However, some studies showed that iVR-based learning activity achieved only similar or even worse learning outcomes (e.g., Moro et al., 2017; Parong & Mayer, 2021) compared to learning activity with other media, such as augmented reality or desktop simulation. These studies typically adopted single-tier multiple-choice questions to evaluate students' performance. Other researchers suggested that iVR may promote different learning outcomes from other media, such as improving 3D spatial understanding (Checa & Bustillo, 2020; Winn et al., 2002). Thus, a better evaluation of students' learning should be adopted to elicit how students could achieve better academic performance with iVR.

Student-generated diagrams have been used to elucidate the level of students' understanding of scientific concepts (Chang et al., 2020). For example, Harle and Towns (2013) showed how drawing tasks could reveal students' understanding of protein structure. Although most of the participants were successful in identifying primary and secondary structures, they were struggling to visualise and explain the molecular interactions that happened in the protein structures. Cooper et al. (2015) also showed that drawing tasks revealed that students have an alternative understanding of intermolecular interactions despite being able to give correct responses to factual questions. With the need to better evaluate the educational benefit of iVR, asking students to visualise their ideas before and after iVR learning tasks may be beneficial.

Students' interactions within iVR environments were rarely investigated. Although more time-consuming, analysis of students' interactions during the learning activity could elucidate dynamics that could not be captured from simple post-tests (Winn, 2003b). More recently, in studies about computer-assisted learning environments, researchers have investigated the moment-by-moment activity of students during the intervention to understand how students used the media. For instance, Cook et al. (2008) reported the influence of prior knowledge on students' use of microscopic and macroscopic chemistry visualisation when working with images on computer screens. Another study showed that group composition was important in driving students' collaborative discussion about physics simulations (Gijlers & De Jong, 2005). Analysis of students' interactions helped to explain why students performed differently after interventions with other media. For example, Yarden and Yarden (2010) showed that student pairs performed better after learning with animation than still images because seeing the dynamics of the molecules promoted the discussion of causal mechanisms. These studies suggest that evaluating students' interactions could help elucidate how students reap the educational benefit of iVR.

In addition to academic performance, many previous iVR studies employed questionnaires to evaluate students' engagement and perceptions of iVR. For example, Bodzin et al. (2021) used a series of perceived immersion and attitude questionnaires. They reported that students perceived iVR activity as useful for learning because they felt more immersed or engaged in the task. While questionnaires are useful to quickly collect students' perceptions in large numbers, they may be limited in helping elucidate the reasons for students' choices (Cohen et al., 2011). Using students' reflections or interviews, some iVR studies reported what students said about their iVR experience (Han, 2020; Southgate et al., 2019): "Fun" and "Engaging" were mostly found in students' comments about iVR. However, apart from the immersive experience, the features of iVR that students perceived as crucial for their learning remained unclear.

Indeed, students could perceive the iVR activity differently from teachers by highlighting different key features of iVR. Dede et al. (2017) identified the key aspects of immersive learning media for inducing learning, which include sensory (e.g., 3D visualisation), actional (e.g., interactivity), narrative (e.g., storylines) and social features. Most iVR studies offered tasks to observe 3D environments or follow a certain protocol to engage students or improve abstract concepts. However, from the student's perspective, the limited opportunity to be analytical and collaborative made these experiences overwhelming. For example, after experiencing a journey into the cells with iVR headsets, students felt enjoyment but were distracted from the learning goals (Parong & Mayer, 2018). On the other hand, few studies have considered a pedagogical approach for learning in iVR environments. For example, limited studies offered students more agency to engage in collaborative, challenging tasks in 3D environments. To address this deficiency, using semi-structured interviews and focus groups, Šašinka et al. (2019) reported students' perceptions of iVR, including how the students identified and overcame the challenges of socially interacting in the iVR environment. Reflecting on these studies suggests that evaluating students' perspectives may help to understand which features of iVR were important and how students use these features for learning.

Some concepts can be learned equally well with other media than iVR, but some concepts, such as those involving dynamic three-dimensional processes, were better understood with iVR (Winn, 2003a). Chemistry, a science about atoms and molecules, can be a good fit for iVR application due to its abstract nature (Hamilton et al., 2020). However, many students deemed chemistry concepts difficult for reasons related to visualisation, context, and language (Johnstone, 1991; Treagust et al., 2000). Chemistry learning can involve changes in chemical reactions that occur as a result of changes in unobservable atoms and molecules. This abstract nature of chemical entities can make it difficult for students to predict the emerging properties of chemical systems (Tümay, 2016). For example, without appreciating how water molecules look and interact in 3D space, students may find it challenging to explain why snowflakes have a hexagonal symmetry (Brini et al., 2017). Such a chemistry explanation also requires students to link various chemistry ideas. However, chemistry concepts were often taught as pieces in class, resulting in students' disconnected understanding of chemistry ideas (Orgill et al., 2019). Furthermore, chemistry ideas were traditionally transferred to students by teachers using chemistry language, which, for novices, may seem abstract and can be misinterpreted (Quílez, 2019). Students then tend to resort to rote memorisation of scientific terms to achieve good examination marks (Hamnell-Pamment, 2023).

Educational iVR applications have been used to help students learn chemistry. In general, most iVR applications in chemistry allow students to experience virtual laboratories or explore 3D molecular structures. Virtual laboratories in iVR have been used as a safe environment for students to improve their laboratory skills (Chan et al., 2021). Nevertheless, existing studies showed mixed results in students' performance after using virtual laboratories (e.g., Dunnagan et al., 2020; Makransky et al., 2019b). The iVR application seemingly does not help students learn, perhaps because the point-and-click interaction does not allow students to improve their procedural skills (Bagher et al., 2020). By exploring simple molecular structures in iVR, students better understand molecular bonding (e.g., Fujiwara et al., 2020) and stereochemistry (e.g., Elford et al., 2021; Miller et al., 2021). However, these simple structures could also be explored using physical models. iVR may be more beneficial for exploring complex molecules or manipulating many molecules to learn concepts that were difficult to explore with other media, such as phase changes (e.g., Gandhi et al., 2020), intermolecular interactions (e.g., Ferrell et al., 2019), or enzyme-substrate reactions (e.g., Bennie et al., 2019; Won et al., 2019).

An educational iVR application can potentially help students learn chemistry. The powerful 3D visualisation coupled with the intuitive interactivity of iVR allowed students to explore 3D molecular structures in situations inaccessible in everyday life. Such exploration can help students understand molecule structures and interactions (Wu & Shah, 2004) and better predict emerging properties of chemical systems (Talanquer, 2011). Instead of simple observation, iVR activities can include challenging tasks relevant to students' everyday lives. Using contextual learning in chemistry helped students to integrate and link chemistry concepts (King, 2012; Nentwig et al., 2007). Instead of exploring the content in iVR individually, students can share the iVR environment with another student. Collaboration can be fostered by providing more complex tasks, resulting in a better understanding of scientific concepts (Nokes-Malach et al., 2019). Communicating with their peers gives students more opportunities to better understand scientific language (Repice et al., 2016).

This study investigated the gap in iVR literature regarding understanding how students use iVR to learn chemistry concepts. Existing iVR studies focused on evaluating students' outcomes and perceptions using simple pre- and post-tests. From those studies, we learned that students perceived iVR as a fun, immersive experience and performed better in recalling declarative knowledge (Hamilton et al., 2020). The reason why students performed better in iVR compared to other media-assisted learning is often unclear. This study fills the gap in the literature by evaluating students' learning interactions and perceptions of iVR compared to magnetic models. Chemistry was chosen as a context in this study because the learning challenges in relation to its abstract nature could potentially be addressed in 3D virtual environments (Merchant et al., 2013). To address the lack of iVR studies that consider pedagogical approaches (Radianti et al., 2020), this study used an in-house iVR application that offered a contextual, collaborative learning experience. An investigation into how students used and perceived iVR applications can better inform future studies on how best to adopt iVR for learning chemistry.

1.3 Aims and Research Questions

The main goal of this study is to identify the educational benefits and limitations of immersive virtual reality (iVR) for pairs of first-year undergraduate students' chemistry learning. The target chemistry concept of this study is hydrogen bonding between water molecules in snowflakes. Students learning interactions, outcomes, and perceptions of their experience were evaluated to address the overarching research question: "What are the educational potentials of immersive virtual reality (iVR) for first-year students' chemistry learning compared to magnetic models?". Magnetic models were used as a comparison to identify the unique educational potentials of iVR. The research questions guiding this study are as follows:

Research Question 1. Concerning students' learning interactions and conceptual changes:

(a) How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions when using *magnetic models*?

(b) How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions within an *immersive virtual reality* environment?

Research Question 2. Concerning students' perceptions of their experience:

(a) How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation when using *magnetic models*?

(b) How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation within an *immersive virtual reality* environment?

1.4 Research Methods Overview

This research investigated the educational benefits of iVR through a qualitative case study research design (Creswell & Poth, 2017). In this study, a case was conceptualised as a pair of students. The participants of this study were 40 first-year students (20 pairs of students) in an Australian university. Chemistry is used as the context, specifically the hydrogen bonding between water molecules in snowflakes. The learning goals identified include hydrogen bonding, simple and complex molecular structures of water, and the formation of the six-fold symmetry of snowflakes. Each pair of students experienced learning activities with magnetic models first before experiencing the iVR learning activity. Before and after each learning activity, we conducted semi-structured interviews with questions about students' learning (through student-generated diagrams and explanations) and overall perceptions of their experience. All learning activities and interviews were videotaped and later transcribed.

Cross-case analyses of students' interactions, learning outcomes, and perceptions of their experience were performed to identify the educational benefits and limitations of iVR compared to magnetic models. For the investigation of students' interactions and learning outcomes, an inductive multimodal analysis (Jewitt, 2013) was adopted to analyse videos of students' interactions, student-generated diagrams, and scientific explanations. The inductive multimodal analysis results of each pair of students were compared to identify any general and unique patterns following a cross-case analysis (Merriam & Tisdell, 2009). For the investigation of students' perceptions of their learning experience with magnetic models and in the iVR environment, a thematic cross-case analysis was adopted to analyse the videos and transcripts of students' interviews. Dede's (2017) immersion features framework was adopted to identify several themes related to key features of iVR from students' interviews.

1.5 Significance

The findings and discussion in this thesis contribute to the educational technology field, especially regarding the application of immersive virtual reality (iVR) for science learning. With the rapid increase in iVR studies, researchers initially relied on simple post-tests to analyse the advantage of iVR for learning. This study offers another way to evaluate the educational benefits of iVR in supporting collaborative chemistry learning. By combining qualitative analyses of students' learning interactions, outcomes, and perceptions of their experience with iVR, this study provides insight into *what* and *how* learning happened or did not happen. The uniqueness of iVR can be elucidated by comparing the extent of students' interactions, outcomes, and perceptions of iVR with magnetic models.

iVR holds the potential to support students engaging in discussion and exploration of 3D molecular structures to establish scientific explanations of natural phenomena. Yet, the benefit of iVR has been constrained to improving students' ability to recall information. To date, there have been limited studies that offer a contextual, collaborative exploration of complex structures in iVR. This study documented and analysed students' conceptual changes and interactions to provide insight into how first-year university students used iVR to learn hydrogen bonding in the context of the formation and shape of snowflakes. Future researchers, educators, and instructional designers may benefit from this study to better understand the unique benefits and limitations of iVR.

Students' perceptions have been useful in understanding the features of iVR that are important for their learning. Adopting the immersive features framework by Dede et al. (2017), this study analysed students' perceptions of their learning experience of the magnetic model and iVR learning activity. The results and discussion of this study may provide deeper insight into how students perceived iVR, including how they approached its key features. Researchers, educators, and instructional designers may wish to consider the relationship between context (target concepts and participants) and the key features of learning media to offer a unique, engaging learning experience with iVR.

1.6 Thesis Outline

This research investigates the educational potential of iVR for students' chemistry learning through evaluations of students' learning interactions, outcomes, and perceptions of their experience. Magnetic models were used to help identify the unique benefits of iVR.

Chapter 2 presents the literature review of current iVR studies in the science education field. Common approaches adopted by existing iVR studies to evaluate the educational benefits of iVR are presented. Requirements for an effective iVR learning experience based on previous studies to address students' challenges in learning chemistry were identified.

Chapter 3 describes the research methods conducted in this study. It explains the rationale for choosing the methodology and provides details of the research designs, participants, learning materials, data collection, and analysis procedures.

Chapters 4 and 5 present the results of the analysis of conceptual changes, interactions, and perceptions of their experience with magnetic models and within an iVR environment. Chapter 4 responds to Research Question 1, while Chapter 5 responds to Research Question 2.

Chapter 6 focuses on the discussions of the educational potentials of magnetic models and iVR identified from the evaluation of students' interactions, learning outcomes and interviews about their learning experience.

Chapter 7 concludes the thesis by providing a summary of the entire thesis that includes the significance, implications for future research, and limitations of the study.

Chapter 2. Literature Review

The main purpose of this chapter is to provide an overview of the status of immersive virtual reality (iVR) research in education, including the research gaps. Three main parts are included in this chapter. The first section presents the overview of virtual reality, from non-immersive to immersive. Known key features of iVR are also elaborated. The second section presents the common approaches to evaluate the educational benefits of iVR, including their limitations. Looking into research in the broader field of science visualisation and computer-supported collaborative learning, alternative ways to evaluate the benefits of iVR are presented. Finally, chemistry education is introduced as the context of this study. This final section presents the main challenges of learning chemistry and how previous iVR studies addressed them. Alternative approaches that could potentially be adopted in iVR and address challenges in chemistry learning are illustrated.

2.1 Immersive Virtual Reality

Virtual reality (VR) has captivated educators because of its capability to immerse students in situations that are impossible to access in real life. Students can swim among human blood cells or fly out to space among the planets. Students can even become someone else and experience a historical event from the perspective of famous figures. A wide range of VR technology is available. Each has different levels of immersion that influence the sense of "being there" in the virtual world.

2.1.1 Types of VR

The term virtual reality (VR) can mean "the sum of the hardware and software systems that seek to perfect an all-inclusive, sensory illusion of being present in another environment" (Biocca, 1992). While VR environments are completely computer-generated, augmented reality (AR) overlaps virtual objects with real environments. Students used devices with cameras (e.g., smartphones and AR goggles) to interact with virtual objects without losing the view of the real environment (Cheng & Tsai, 2012).

Virtual reality technology ranges from non-immersive to immersive. Non-immersive VR, commonly known as desktop virtual reality (DVR), displays the virtual environment on a 2D screen.

When using DVR, users interact with the virtual environment using a mouse, keyboard, or joystick (Di Natale et al., 2020). Cave Automatic Virtual Environment (CAVE) envelops students in a room covered by screens (on the walls and floor) that display the virtual environment. Inside the CAVE, students wear special glasses for a stereoscopic view of the virtual environment (Limniou et al., 2008). Some researchers consider CAVE an immersive VR (Jensen & Konradsen, 2018). However, in this study, CAVE is considered non-immersive because it does not completely block out the visual of the real environment (Radianti et al., 2020).

Immersive virtual reality (iVR) uses the head-mounted display (HMD) device, or the iVR headset, to completely replace the visual of the real space with virtual space. HMD devices emulate a stereoscopic display of a computer-generated world, creating the illusion of 3D depth. The users' body movements are synchronised with the movement inside the virtual environment, allowing intuitive interactivity (Slater & Sanchez-Vives, 2016). Types of HMD devices commonly used in educational contexts include high-end iVR (such as HTC Vive, Oculus Rift, and PlayStation VR), standalone iVR (such as Lenovo Mirage Solo, Oculus Quest, Oculus Go, VIVE Focus), and mobile iVR (such as Samsung Gear VR, Google Daydream, Google Cardboard) (Stojšić et al., 2019).

High-end iVR headsets require a separate computer (PC) to run the data processing, such as graphics rendering. The headsets are usually tethered to the PC using a cable (Rendevski et al., 2022). With a powerful PC, this type of iVR headset can accommodate complex and advanced virtual environments. It has a wider field of view (FoV) and user-tracking compared to other kinds of HMD. High-end iVR headsets were predominantly used in higher education research settings (Radianti et al., 2020). Some previous studies (e.g., Won et al. 2019) were even able to bring multiple users together in a shared virtual environment using high-end iVR headsets. However, high-end iVR, which is generally heavier, may affect users' comfort if used for a prolonged time. Users' movement can also be limited because of cables (Angelov et al., 2020). Also, using a wireless adapter to replace the cable can greatly improve users' freedom to move in the virtual space.

Standalone iVR headsets have all the computing components required to generate the virtual environment without needing a separate PC. The sensors are in headsets to track users' movements. Without being tethered to a desktop computer, the users have higher mobility to interact with the virtual environment (Angelov et al., 2020). However, the computational power is limited compared to high-end iVR, restricting it to displaying a simpler iVR experience.

Mobile iVR headsets are iVR glasses without any built-in computer hardware and work in conjunction with a smartphone that can be slipped in front of the lenses of a mobile iVR headset. Like standalone iVR, mobile iVR is lighter and easier to set up. It is also considered the cheapest type of HMD. The visual of the virtual environment and user tracking is limited due to the computational power of the smartphone. Unlike other types of HMD, mobile iVR generally does not work with controllers that allow a wider range of interactions (Angelov et al., 2020). Users typically interact with the virtual space simply by turning their heads.

2.1.2 Features of iVR

The technological advantages that make iVR unique are its *immersion* and ability to promote *presence* (Slater & Sanchez-Vives, 2016). Immersion refers to the capability of a computer to display an illusion of reality. Immersion is considered a technological attribute and can be assessed objectively. In contrast, presence refers to the personal experience of being in an environment, even though the physical body is in another (Slater & Wilbur, 1997). The technological requirement for a higher degree of immersion includes a wide field view of the environment, ideally 200 degrees horizontally and 120 degrees vertically, tracking of the student's body, and no lag in responding to the student's input/interaction in the virtual environment (Slater & Sanchez-Vives, 2016; Winn, 1993). It was assumed that with a higher fidelity of representation and a higher degree of freedom to manipulate the virtual objects, immersion would increase, and consequently, students' sense of presence (Dalgarno & Lee, 2010).

Previous studies proposed that increasing students' sense of presence could result in improvement in their learning (Grassini et al., 2020). According to social constructivist theory, students learn by interacting with the environment and other people (Vygotsky & Cole, 1978). When presence is achieved, students are more likely to interact/behave realistically in an iVR environment and construct meaning from those interactions (Slater, 2017). With iVR, the intangible phenomena can be reified for students' multisensory explorations and meaning-making processes (Salzman et al., 1999). Therefore, iVR is particularly attractive for teaching concepts that were difficult to access or imagine in real life (Freina & Ott, 2015).

Identifying the key features of iVR can help researchers to understand how students interact in iVR environments. Dede et al. (2017) identified four immersion features: sensory, actional, narrative, and social. Won et al. (2023) further elaborated the features into technological (sensory and actional) and pedagogical (narrative and social) features.

The *sensory feature* is a technological feature that influences the sense of spatial presence through multisensory stimulus. Spatial or physical presence refers to a sense of being in the environment (Lombard & Jones, 2015). The multisensory stimuli that influence the fidelity of representation of the virtual world include the 3D visual display of the iVR environment, 3D spatial audio, and haptic feedback. The 3D visual display encapsulates students in a “realistic” virtual world, making them suspend their perception of the real world (Slater & Sanchez-Vives, 2016). The source of audio inside the virtual world can be programmed as if it comes from different directions and distances to increase students’ spatial presence further (Slater, 2009). Haptic feedback provides spatial presence through touch (Dede, 2009).

The *actional feature* refers to technological features influencing a sense of spatial presence through intuitive interaction. An iVR system recognises students’ movements as input, which allows them to manipulate virtual objects and feel that their actions are realistic and have real consequences (Slater, 2009). Students’ interactions with the virtual environment can be simple through eye-gazing, select-and-click, or more complex through hand or full-body movements. The synchrony between representational fidelity (sensory) and students’ interactions (actional) can induce students’ sense of presence (Cummings & Bailenson, 2016).

Considering the technological capabilities of different HMD devices, we can assume that high-end iVR can induce a higher sense of presence than mobile iVR. However, after a closer look at the features of iVR systems, previous studies reported that the combination of user-tracking and wider fields of stereoscopic visual was more crucial to inducing a sense of presence than the quality of the graphic, audio, or haptic (Cummings & Bailenson, 2016). Providing a high fidelity of the virtual environment through good graphics, audio, and haptic qualities is beneficial to help students feel that they are in another space. However, these sensory spatial cues should be backed up by the ability of the VR system to recognise and respond to students’ physical actions (students’ interactions). This two-step process – spatial cues and experience of self in the place – is required to determine students’ presence, specifically a sense of physical or spatial presence (Wirth et al., 2007).

The *narrative feature* includes pedagogical approaches for intellectual and emotional engagement of the experience. Students can be immersed in the virtual environment through narrative immersion by incorporating engaging content or storyline (Slater & Wilbur, 1997). For example, students could embody the role of Lenin giving a speech in 1920 Moscow to maximise their engagement in the history of the Russian Revolution (Slater et al., 2018).

The s*ocial feature* refers to pedagogical approaches to induce social presence – a perception that other beings coexist and react to you (Kreijns et al., 2022; Lee, 2004). Social presence stemming from interactions with other social beings, such as human or pedagogical agents (Veletsianos & Russell, 2014), can captivate students in the shared virtual space (Krämer, 2017). For example, autistic children could train their communication skills by interacting with virtual classmates with different personalities and feel as if they are talking with real classmates (Herrero & Lorenzo, 2020).

One of the learning theories that aligns with the *narrative* and *social* immersion aspects of iVR is social constructivism (Dede et al., 2017). Constructivism, specifically social constructivism, proposes that learners actively build knowledge by interacting with the environment and other people (Cakir, 2008; Vygotsky & Cole, 1978). The proponent of this learning theory gives the learners an active role in making meaning from their current experience while reflecting on their prior experience. The learning approaches to accommodate the social constructivist perspective differ from a traditional instructional system that only puts an active role on teachers (Jonassen, 1991). Learning approaches stemming from social constructivism include contextual or situated and collaborative learning. Situated learning provides students with the context related to *narrative*, while collaborative learning is related to *social* immersion.

2.2 Evaluation of the Educational Benefits of iVR

Research about virtual reality (VR) spans decades and started with its application to train fighter pilots (Coburn et al., 2017; Dede et al., 2017). Virtual reality studies comprise many types of VR, from non-immersive to immersive, as presented earlier. Due to issues such as cost and logistical challenges, iVR was mainly used inside expensive laboratories. The recent development of lighter and more affordable iVR headsets made iVR technology more accessible for many researchers. Consequently, most of the iVR research focused on exploring whether students who experience iVR could achieve better learning outcomes. These studies generally reported positive outcomes in terms of learning motivation and simple declarative knowledge (Matovu et al., 2022; Wu et al., 2020). A shift towards a more in-depth evaluation of cognitive skills in addition to affective measures is more noticeable in recent iVR studies but is still limited.

In the following sections, common approaches to evaluate the benefit of iVR are presented. In general, the use of iVR for education was evaluated through students' conceptual changes and students' perceptions. For the evaluation of conceptual changes, researchers tend to rely on knowledge tests given before and after the iVR intervention (see Section 2.2.1). An alternative way to evaluate the benefits of iVR is by analysing students' interactions (see Section 2.2.2). In addition, approaches to evaluating students' perceptions of iVR are described (see Section 2.2.3). For each type of evaluation of iVR, examples of notable iVR applications and their key features were also illustrated.

2.2.1 Evaluation of Students' Learning Outcomes Pre/Post-iVR

Other iVR studies implemented knowledge tests to better understand what students learned from their iVR experience. Depending on the goal of the iVR application, the knowledge test can include tests for procedural knowledge or declarative knowledge. Procedural knowledge consists of the knowledge to perform a technique or method (know-how), for example, building a house, driving, or performing DNA extraction (Anderson et al., 2001). On the other hand, declarative knowledge encompasses factual and conceptual knowledge (know-what) related to basic elements of the discipline and its relationship (Anderson et al., 2001).

Evaluation of Procedural Knowledge. Evaluation of procedural knowledge is typically done after iVR intervention by a paper-based or skill test. Dunnagan et al. (2020) used sets of questions asking students to identify and explain the steps or certain aspects of the procedures. They reported that students' written explanations of the procedures after iVR intervention were slightly better than in traditional laboratory settings. Other researchers evaluated procedural skills with behavioural transfer tests. For example, after the iVR experience, students were asked to perform a first aid response to an accident in the laboratory (Makransky et al., 2019a), build a real wall frame (Osti et al., 2021), perform a cadaveric task such as a dissection (Lohre et al., 2020), or assemble a complete circuit (Nie & Wu, 2020). From the behavioural transfer tests, these studies reported better task performance, including the speed in performing tasks and the ability to solve problems in real laboratories after learning the required skills in iVR-based learning activities.

iVR experiences designed to develop procedural skills generally allowed students to perform basic interaction with the environment (Radianti et al., 2020). Using iVR, students can practice procedural skills with minimal hazard risk and cost. Instead of simply observing the virtual environment, students can decide the next actions to manipulate in the environment. In general, students can practice the technique repeatedly without worrying about logistical and ethical issues with iVR (Hamilton et al., 2020). Ideally, iVR for procedural or psychomotor skills allows students to do more interaction, resembling the actions they could perform in a real-life situation (Jensen & Konradsen, 2018).

The iVR learning experience for procedural skills usually puts students in a role of a certain profession and prompts them to perform the techniques. For example, students can choose the next steps to complete a chemistry laboratory protocol in iVR (e.g., Makransky et al., 2019a). Their choices determine the results of the laboratory experiment. Students can also act out the procedure to practice their skills, mostly by moving their hands. For instance, students acted out the surgical procedures (Lohre et al., 2020). Limited studies detected students' full bodies to allow more natural interaction inside the virtual space. In an engineering study, for example, students built framed wall components inside iVR by performing actions that included measuring the wood and hammering the nails (Osti et al., 2021). Providing students with more technological features (free movement, haptic) may help them practice their procedural skills more effectively in iVR (Coban et al., 2022).

The iVR applications for procedural knowledge or skill training are ideally evaluated by giving a skill test. Apart from the ones mentioned above, iVR studies for procedural knowledge typically evaluated the benefit of iVR only through students' perceptions of the learning experience or through the evaluation of declarative knowledge (Matovu et al., 2022; Radianti et al., 2020).

Evaluation of Declarative Knowledge. Declarative knowledge was typically evaluated through pre-post-tests, including multiple-choice or short open-ended items. In most cases, the questions evaluated students' ability to recall information. In iVR studies for medical anatomy, the knowledge test comprised multiple-choice questions, such as "Which bone of the skull contains the middle portion of the ear?" (Moro et al., 2017). Some studies evaluated knowledge retention, but again, the items used concerned the recall of factual knowledge (e.g., Gloy et al., 2022). The declarative knowledge tests of previous iVR studies commonly resulted in positive results (Matovu et al., 2022). However, when iVR-based learning was compared with other media such as AR, desktop simulation, or tablets, the results of declarative knowledge tests were moderately positive (Wu et al., 2020), and small numbers of studies even showed negative effects (Makransky et al., 2019b).

Short-answer or single-tier multiple-choice questions have been a popular choice to evaluate students' achievement before and after iVR. The questions can be arranged to test a wide range of topics, and the answers can be marked rather quickly (Towns, 2014). However, students can excel in multiple-choice or short-answer questions by algorithmic means (Hartman & Lin, 2011) or by rote memorising scientific definitions (Nahum et al., 2004). Two-tier multiple-choice questions have been used to better assess students' level of understanding by asking students to justify their choices (Chandrasegaran et al., 2007). Yet, multiple-choice questions were not able to evaluate students' underlying understanding of some concepts, especially the ones about how molecules interact at the particulate level (Kern et al., 2010).

Asking students to create their own representation may give insight into how they conceptualise the ideas, especially the spatial information that may be difficult to externalise through writing or speech (Harle & Towns, 2013). For example, both Meyer et al. (2019) and Thompson et al. (2020) evaluated students' declarative knowledge of cells' organelles after using iVR. Using the multiple-choice test, Meyer et al. (2019) reported which organelle students remembered and did not remember. Using drawing as a post-test, Thompson et al. (2020) reported students' recall as well as how students conceptualise the cellular environment. From the drawings, students showed a better appreciation of the different shapes and sizes of the organelles as well as the density of the cellular environment. However, previous iVR studies in chemistry have not yet implemented drawing tasks to evaluate students' knowledge gain.

Students were often tested for their understanding of scientific terms. Yet, such tests were ineffective in revealing students' challenges in applying scientific terms in a context and visually representing concepts at the submicroscopic level (Nyachwaya et al., 2011). For example, previous studies showed that even though students knew the definition of *hydrogen bonding*, most of them did not necessarily know how water molecules interact with each other (Matovu et al., 2023a; Nahum et al., 2004). To address this gap, prompting students to draw and conceptualise chemistry terms encouraged them to organise their knowledge and decide on relevant information and the most suitable way to represent their conceptual understanding (Ainsworth & Scheiter, 2021).

However, drawings should be used cautiously as certain concepts, like dynamic interactions, can be more effectively conveyed verbally or in writing. Conversely, spatial and composition elements (e.g., polarity and structures) can be better represented as drawings (Kunze & Cromley, 2021; Ryan & Stieff, 2019). In some cases where students struggled to articulate a term to explain phenomena, hand gestures were used to aid students' explanations (Ping et al., 2021).

A wide range of learning approaches has been used to improve students' declarative knowledge in iVR. The most common iVR application for declarative knowledge involved providing students with a first-person view and natural manipulation of 3D structures. This approach allowed them to better understand 3D spatial information. Cells and molecules are considered abstract because they cannot be seen through the naked eye. With iVR, students can visit these abstract realms, visualise them better, and conceptualise the information better. For example, students can rotate and observe the cells (Meyer et al., 2019), the moon (Madden et al., 2020), or human anatomy (Ekstrand et al., 2018) to get information about those structures. The structures can be simple and complex, such as the interior of the cells (Thompson et al., 2020), an enzyme-substrate structure (Bennie et al., 2019), or an entire ancient town (Checa & Bustillo, 2020). By evaluating students' declarative knowledge through means beyond single-tier multiple-choice questions, the unique benefit of iVR for learning could be understood.

2.2.2 Evaluation of Students' Interaction in iVR

Most iVR studies evaluate the learning benefits from pre and post-tests. The learning interaction during the iVR activity was often considered a "black box". Thus, the reasons why students learned or did not learn could not be clearly ascertained (Winn, 2002). Students' interactions in a learning environment are complex and cannot be reported by a simple causal explanation (Turner & Christensen, 2020). Different patterns of student interaction may arise depending on students' characteristics, the design of the learning environment, or other variables (Janssen et al., 2010).

Compared to iVR studies, there are many more studies of computer-supported learning environments that have investigated students' interactions during the learning activity. These studies investigated student-content/tool interaction to better understand how technology can augment face-to-face interactions or transform them into different modes of engagement (Dennen & Hoadley, 2013). For example, a case study by Enyedy et al. (2015) showed how elementary students moved their bodies in relation to virtual objects to reason about friction during an augmented reality (AR) learning activity. By analysing student-content interaction, these authors suggested that allowing students to perform embodied action and reflect on it was beneficial for students' learning with AR. However, it was also important to acknowledge that students may interact differently within the technology-supported environment. For instance, Klopfer and Squire (2008) followed the interactions of several students with an AR simulation. They found that students used different elements of the simulation depending on the students' learning strategies and beliefs. Students who focused on the social aspect of the questions used the interviewing features of the application. On the other hand, students who saw the questions as mathematical problems tended to use the GPS sampling feature. These studies also showed that a more in-depth examination of the interaction of several groups of students helped previous researchers identify the pedagogical and technological elements that should be considered in their computer-based learning activity.

Many studies included collaborative aspects in their computer-assisted learning environments to enhance learning (Chen et al., 2018). These studies analysed social interaction (student-student or student-teacher) in addition to student-content/tool interaction to understand how technology supported students' collaborative learning. For example, Zenouzagh (2023) compared the patterns of student-student interaction in text-based and multimedia computer-assisted learning activities. They showed that the aid of audio and visuals engendered more collaborative interaction patterns. In contrast, students adopted a more expert-novice role in the text-based learning activity. In another study by Velamazán et al. (2023), students demonstrated an increase in collaboration by offering more feedback when their identities were kept anonymous. These examples of research findings showed that technology features can influence how students interact with each other.

Although quite scarce, some educational iVR studies evaluated students' interactions. These studies typically implemented more sophisticated interactivity or provided social features in their iVR applications (e.g., Price et al., 2018; Sugiyama et al., 2021). For example, Price et al. (2020) allowed students to walk around the virtual space to learn about Cartesian coordinates. Their students' interactions analysis explained the link between embodied actions and students' learning of geometry. The researchers found that students engaged in perspective-taking when discussing strategies to complete the task in iVR. Without understanding each other's point of view, the pairs took longer to complete the task. They also used the position of their own body as a reference to point out spatial information to their peers. Both studies showed how spatial awareness and perspective-taking influence students' collaboration in iVR activity. Yet, the details of the interaction process were often reported independently from the knowledge gained.

Analysis of students' interactions can help researchers better understand how the students achieve the learning outcomes. Šašinka et al. (2019) put two students in the same iVR space and analysed videos of students' interactions and their perceptions of iVR experiences. They reported students' motivation to learn was influenced by having their peers in the iVR space. The students invented a new way of communication inside iVR using gestures due to the "faceless" avatars. While Šašinka et al. (2019) described students' interaction in iVR, it would be interesting to see how different students' interactions in iVR compared with other media. By comparing the interaction with different media, the unique benefits of iVR could be unravelled. However, to date, comparison iVR studies typically reported pre and post-test results instead of analysing students' interactions during the learning activity (e.g., Brown et al., 2021; Makransky et al., 2019b).

2.2.3 Evaluation of Students' Perceptions of iVR

Students' perceptions of the learning environment can influence how they learn (Struyven et al., 2005). For example, students who perceive university as an environment with heavy workloads tend to have surface approaches to study, while students who see the campus as a good teaching environment have a deep learning approach (Lizzio et al., 2002). The majority of iVR studies evaluated students' or teachers' perceptions of the experience, including presence, engagement/enjoyment, motivation/self-efficacy, attitude, and perceived usefulness (Matovu et al., 2022). Most iVR studies used self-rated Likert scale surveys delivered after the iVR experience (Di Natale et al., 2020). In general, students and teachers gave positive reviews on their iVR experience. But, when compared to other media, students' self-efficacy was not significantly different (e.g., Huang, 2019; Moro et al., 2017). The Likert scale survey gave an overview of students' perceptions, but the reasons behind their ratings and how it affected their learning were often unclear.

Some iVR studies used qualitative approaches to better understand students' perceptions using interviews (Cheng, 2021) or written self-reflection (Han, 2020). From the comments of participants, these studies generally identified 3D visualisation as the main benefit for students' learning. Students feel a sense of presence by getting a 360-degree view of the virtual world. Their comments include "It is so real" (Han, 2020) or "Cool! The scenes seem to have a 3^{rd} dimension" (Cheng & Tsai, 2019). Increased motivation and perceived learning can come from novel experiences, such as being able to situate oneself in a realistic environment or convenience. For example, students commented, "It (VR) gives me an opportunity to learn stuff without having to go to the actual place" (Klippel et al., 2019). From teachers' perspectives, students were more motivated to engage in class and learned better after iVR. For example, a participant commented, "More details of scientific phenomena are included in iVR for enhancing abstract concept understandings." (Cheng, 2021). It was clear that the iVR technological aspect was important for students' learning engagement. However, it is also important to identify the pedagogical aspect from student interviews. As pointed out by many educational researcher, students' learning experience were shaped by the combination of the medium, instructional method, and the learners' characteristic (Lui et al., 2023; Mikropoulos & Natsis, 2011).

In the field of educational technology, students' perceptions have been analysed to help researchers identify key features of new learning media. Although not yet applied in iVR studies, a theoretical framework can be adopted to identify key benefits of a computer-supported learning environment from students' interviews. So and Brush (2008) adopted Moore's three types of interactions to analyse students' perceptions of a blended learning environment. Using the interaction framework, they could identify three critical factors (course structure, emotional support, and communication) that affect students' perceptions of online learning activities. In another research about online writing systems (Chong, 2019), the author used a tripartite conceptual framework for written feedback. The author identified key functions of the system, including the learning process, depending on how students perceived the written feedback. These studies gave an example of how not only technology aspects, but also pedagogical aspects of technology-assisted activities can be identified from students' interviews. This approach of using a framework to analyse students' perceptions could also be adopted in iVR studies.

Studies that evaluated students' perceptions generally used iVR to promote students' learning experiences by "transporting" them to another place (Freina & Ott, 2015). Students observed the virtual environment by turning their heads and felt they were visiting another place without leaving their classroom. Mobile or standalone HMDs were generally used because they were cheaper and could be easily used by many students in a classroom setting at the same time. For example, several elementary students used iVR in class to make a virtual field trip to historical sites (Cheng & Tsai, 2019) or natural parks (Han, 2020). Students can also visit another realm, such as the molecular level (Gandhi et al., 2020) or the interior of human cells (Huang, 2019). A teacher was typically present in the class to assist students in their virtual world exploration and gave verbal guidance (e.g., Gandhi et al., 2020). Apart from looking around, students typically have minimal interaction with virtual environments. From the evaluation of students' perceptions, these studies reported the benefit of iVR in terms of learning engagement.

2.3 iVR for Learning Chemistry

Educational iVR applications have been used in various discipline areas. So far, iVR has been more effective for areas that require an understanding of spatial arrangements and abstract information (Coban et al., 2022; Hamilton et al., 2020). This study considers chemistry to be a topic that can potentially be learned effectively with iVR.

Understanding chemistry can help us explain how natural phenomena that we observe in everyday life happen. Chemistry essentially deals with the structure, composition, properties, and reactions of substances – the building blocks of our world. Yet, many students found chemistry difficult to comprehend (Treagust et al., 2000; Tümay, 2016). Students felt less motivated to choose science subjects, especially chemistry. Students also often do not see the relevance of chemistry concepts in their everyday lives, which affects their self-efficacy in chemistry (King, 2012). Many schools have incorporated laboratory practicums so that students can perform protocols and feel confident as novice chemists (Hofstein, 2004). While laboratory experiments allowed observations of the results of chemical reactions, the underlying mechanism of how and why those reactions happened may seem abstract for students. Chemistry topics (e.g., intermolecular forces, kinetics, acid and bases, thermodynamics, etc.) were often learned separately using newly coined chemistry terms, which makes it difficult for the students to link the concepts and explain natural processes (Osborne, 2002; Wu, 2003). The following section illustrates students' main challenges in learning chemistry and how iVR could potentially address those challenges.

2.3.1 iVR for Exploring Abstract Chemical Entities

Challenges in Learning Chemistry. Chemical entities – atoms and molecules – cannot be seen through the naked eye; thus, they are typically represented as a model for communication and exploration purposes (Coll, 2006). For chemistry classes, the scientific models are typically in the form of text, symbols, or pictures. When students learn chemistry, they need to understand the purpose of the models and interpret these models (Gilbert, 2004). For example, H_2O has two hydrogen atoms and one oxygen. The interpretation does not stop there. H_2O also means a water molecule. Students may learn the properties of hydrogen and the properties of oxygen, but the properties of water molecules are not simply the addition of hydrogen and oxygen. Like most other molecules, the properties of water molecules are also determined by the configuration and interactions of the constituent atoms. It may be challenging to explain emerging chemical properties by only relying on the addition of symbols without an appreciation of how the molecules look (Tümay, 2016).

Appreciation of molecular configuration and interactions comes from students' mental models (Wang & Barrow, 2011). From a constructivist perspective, students develop their mental models from their everyday experiences. However, atoms and molecules are submicroscopic entities that may be difficult to experience directly in students' daily lives (Gilbert & Treagust, 2009). From imagining these abstract entities, students may develop a mental model that is different from widely tested and accepted scientific models (Coll & Treagust, 2003). When students face challenges in conceptualising the abstract concepts of chemistry, they tend to resort to rote memorisation of facts and formulas (Nyachwaya et al., 2014). This issue of rote memorisation was augmented by the focus on passing a matriculation exam, which often can be solved simply through algorithmic strategies (Tsaparlis et al., 2018).

Visualisation has been used in chemistry lessons to assist students in constructing their mental models to be as close to the scientific models as possible (Gilbert, 2004). Pictorial visualisation gives a better idea of molecular structures. It can show the amount, position, and size of each atom in a molecule. However, 2D visualisation lacks depth cues, making it challenging for students with low spatial skills to comprehend. 3D visualisation of atoms and molecules can help students better develop their mental model of molecular structure (Wu & Shah, 2004). Previous studies have used physical models to show molecular structures in relation to stereochemistry and bond polarity (Stieff et al., 2005). With the 3D structures in front of them, students did not have to deal with the ambiguity of text symbols or other 2D visualisations. Yet, previous applications of physical models have often been limited to showing single, simple molecular structures (Stieff et al., 2016; Stull et al., 2013). Computer simulation has been used to show complex molecular structures (Jenkinson & McGill, 2012), but again, it is still a 2D display that lacks depth cue.

iVR to Address the Challenge. The sensory and actional features of iVR could be capitalised to allow students' exploration of 3D molecular structures. Unlike physical models and computer simulations, iVR provides immersive 3D visualisation of complex molecular structures. The abstract chemical entities are reified as "realistic" 3D objects in iVR (Winn, 2002), which means the spatial arrangement of each atom in a molecule is made explicit for students. By observing the molecular structure in 3D, students can appreciate the importance of chemical configuration and interactions in chemical reactions (Bennie et al., 2019). For example, students can observe the position of methane molecules in a carbon nanotube in iVR. Their observations resulted in an appreciation of spatial arrangements and size in chemical reactions and allowed them to predict which molecules could fit the nanotube (Ferrell et al., 2019). Such observations of 3D spatial arrangements were difficult to make in other media.

Students engage with their prior knowledge when they try to represent their ideas (Wang & Barrow, 2011). They need to organise the relation of the concepts and select which concepts to represent. In the process of organising and selecting their prior knowledge, students can develop new links and a new understanding of the concepts (Tytler et al., 2019). In this sense, students can learn more when they create their own visualisation (Wu & Rau, 2018; Zhang & Linn, 2011). Yet, alternative learning methods, such as building physical models or gesturing, could be better than learning by drawing for some concepts involving complex 3D structures or dynamic systems (Ainsworth & Scheiter, 2021).

Active construction of visualisation could lead to better learning performance than simply observing visualisation (Naps et al., 2002; Roberts et al., 2005). Instead of passively viewing 3D molecular structures, students can pick up an atom or a molecule and build their own 3D molecular structures in iVR. In an iVR environment, students are no longer restricted by the 2D plane and the logistic issue (e.g., instability of physical models). Unlike laboratory experiments that deal with macroscopic observations, students can deal directly with the molecules in iVR. When students manipulate the reified chemistry concepts in iVR, they can test their ideas, observe the conflict (if any), and revise their ideas to construct a better mental model of chemistry concepts. For example, students can integrate the concepts of electron density and 3D structural aspects after experimenting with enzyme-substrate molecular configurations in iVR (Won et al., 2019).

2.3.2 iVR for Contextualising Disconnected Chemistry Ideas

Challenges in Learning Chemistry. With the development of the chemistry body of knowledge, chemistry textbooks contained more topics than ever. First-year or introductory chemistry was typically designed as a survey of the discipline (Cooper et al., 2017a). As a result, the introductory chemistry curriculum tends to be overcrowded (Ho, 2019). Students were expected to continue the course to the next level in order to get a deeper understanding of the chemistry topics. However, without motivation to continue the course, these students would have no opportunity to develop a coherent mental model of the chemistry concepts (Cooper et al., 2017a).

Chemistry phenomena are complex, and their explanations involve the interlink of many levels of chemistry ideas (Talanquer, 2018). The sheer amount of chemistry ideas and complex phenomena may overwhelm students and affect their self-efficacy in completing chemistry courses (Cooper et al., 2017a). Reductionist approaches have been used in chemistry classrooms to make complex chemistry phenomena accessible to students. According to reductionist perspectives, complex phenomena can be learned by analysing their simpler components. Each topic (e.g., bonding, reactivity, acidity, thermodynamics, etc.) was delivered to students as context-free facts (Orgill et al., 2019). These chemistry topics were often taught as separate chapters, resulting in students developing a fragmented understanding of chemistry. The aggregations of isolated topics without a clear strategy on how to connect them can lead to low learning motivation (Gilbert, 2006). Although reductionist approaches helped students cover many chemical terms, students found difficulty in applying or transferring the knowledge in a new context or real-life situation (Ho, 2019).

Reductionist approaches suggested that teachers transfer each silo of concepts to students so that they could later understand the concepts as a whole (MacInnis, 1995). The consequence of this approach was the interlink between the silos of concepts was often overlooked (Orgill et al., 2019). According to the constructivist view, information cannot be remembered as an independent abstract unit (Bednar et al., 2013). Students learn about an idea when they learn it in the context where the ideas are used. For example, students can perform experiments with a dissolved oxygen kit in the laboratory to learn about solvation. Even though the previous example situated students in a laboratory, the context can seem superficial. In a non-authentic scenario, students' learning may only focus on remembering and performing a protocol instead of linking concepts to solve complex issues (Sadler, 2009).

iVR to Address the Challenge. The narrative features of iVR (task design and storyline) could be implemented to engage students emotionally and intellectually. For example, students can become white blood cells patrolling the blood vessels and defending the body from incoming pathogens (Zhang et al., 2019). By including a storyline or context, students' learning was not only restricted to gaining information (e.g., about structures). The context helped students to link various ideas. For example, Barab et al. (2007) let students work with environmental experts trying to solve a problem with the decline of fish populations. In this context, students not only learned the protocol to measure dissolved oxygen in a water sample but also gained a new perspective on applying and relating their learning to other branches of science. Studies in computer-assisted learning showed positive outcomes in relation to situated learning (Dawley & Dede, 2014).

Although the application of situated learning approaches is still rare in iVR, the few studies reported have shown positive perceived learning outcomes (e.g., Bibic et al., 2019; Zhang et al., 2019). For example, Sugiyama et al. (2021) situated the learning of anatomy for surgery preparation. Trainee surgeons discussed their exploration of patients' 3D brain imagery with senior surgeons. By having an authentic task (surgery preparation), these trainees were shown to have improved their understanding of patient-specific anatomy and their ability to transfer their learning by correctly diagnosing several other illustrative cases in the post-test.

Situated learning has been adapted in chemistry lessons to motivate students (King & Ritchie, 2012) and help students develop a comprehensive understanding of chemistry ideas that allow them to explain natural phenomena (Wu, 2003). In situated learning, students are typically faced with complex real-life problems (Dawley & Dede, 2014). As they formulate the explanation of complex issues, students begin to gain a better understanding of the basic ideas and connect these ideas (Nentwig et al., 2007). Constructivist learning approaches have been implemented in a traditional classroom, but the introduction of technology has made the implementation easier (Wang, 2009). The iVR learning tasks can be woven into a captivating narrative that motivates students to complete the task. The narrative can be in the form of a complex real-life situation that prompts students to link basic chemistry concepts.

Students may find complex real-life problems inaccessible and may require support to complete the task. Students generally try to find a correct answer instead of exploring various ideas to explain a phenomenon (Broman & Parchmann, 2014). To avoid being overwhelmed by complex tasks, students can be prompted to approach the issue by starting with basic chemistry knowledge. A simple structural model can be presented as a starting point for students to anchor their explanation of the complex issue (Broman et al., 2018). As shown by Broman et al. (2018), without scaffolding, only a few students can reach a higher level of explanations of complex problems. A series of prompts to scaffold students can be embedded in the iVR learning experience as they link more concepts and solve complex problems.

2.3.3 iVR for Making Chemistry Language Meaningful With Peers

Challenges in Learning Chemistry. Chemistry ideas, like other scientific ideas, are communicated through language. The goal of science education is to help students use the language of science to construct and interpret meaning (Osborne, 2002). The language of science, including chemistry language, is unique compared to everyday languages. Words used in chemistry are polysemous as it has a different meaning from everyday use (Quílez, 2019). Students need to be aware of the context when using certain scientific terms. For example, *polar* (molecule) in chemistry can be explained as a molecule with an unsymmetrical electron charge distribution. Yet, some students held the everyday meaning of chemistry terms by explaining *polar* molecules as cold, positive, and negative in relation to the south and north poles (Song & Carheden, 2014). Moreover, many technical terms used in chemistry are rarely used in students' everyday lives (Markic & Childs, 2016). For example, *electronegativity, chiral,* and *entropy*. Without having encountered it before in everyday situations, these newly coined chemical terms may seem abstract to students.

Using the correct chemical terms in the right context does not always indicate that students understand the meaning (Levy Nahum et al., 2007). For example, most students were able to recall the definition of chemical terms but were unsuccessful in using them to decide the correlation between the terms (Tsaparlis et al., 2018). Another study also showed students' usage of algorithms to successfully solve chemical problems (BouJaoude et al., 2004). But when the students were given another new context (Nyachwaya et al., 2014) or asked to show their reasoning at a particulate level (Kern et al., 2010), their rote memorisation or algorithm strategy often failed.

For students to understand the meaning of scientific terms, they must use their own words to express chemical ideas instead of directly recalling their definitions (Osborne, 2002; Quílez, 2019). Yet, students generally did not have enough opportunity to talk about chemistry in class. In teacher-led chemistry classes, students typically memorise the chemical terms told by the teachers or textbook (Bleicher et al., 2003). The focus on having a correct definition could come from teachers' and students' perceptions of the time constraint to cover many topics and the pressure to excel in the examination. Most examinations test students' ability to recall scientific terms. Such closed or short-answer questions could cloud the assertion of students' limited capabilities to explain the meaning of those scientific terms (Osborne, 2002). Learning approaches that engage students in scientific discourse are needed to help students use and understand chemistry language beyond remembering scientific terms and solving basic algorithm problems (Bleicher et al., 2003).

iVR to Address the Challenge. The social feature of iVR could be considered to engage students in meaningful scientific discussion. With the advances in iVR technology, more than one student can occupy the same virtual environment. Sharing the same virtual space allows students to talk to each other to discuss what they observe and experience inside the virtual space. Having *symmetry* by giving students equal access to the virtual environment (including sharing the 3D virtual objects) can foster collaborative learning (Rummel & Spada, 2005). As shown in a previous iVR study, students were engaged with their peers when completing a common task in the same iVR space (Šašinka et al., 2019). For chemistry, an off-the-shelves application, Nanome VR, was typically used (e.g., Fombona-Pascual et al., 2022; Qin et al., 2020). This application allowed two students to explore a 3D protein structure and discuss it in relation to protein-drug interactions.

In a collaborative learning environment, students can practice using scientific language to articulate their ideas to their peers (Repice et al., 2016). Collaborative learning refers to a situation wherein a specific type of interaction between students is anticipated to stimulate learning (Dillenbourg, 1999). Instead of ensuring students remember the definition of each scientific term, science education is more interested in helping students understand the meaning of the terms and use them appropriately. Previous studies suggested that students internalised the meaning of scientific terms when they were able to use their own words to elaborate on them (Brown et al., 2010; Quílez, 2019). When collaborating with their peers, students tend to use everyday language to express their ideas (Song & Carheden, 2014). Thus, iVR that supports collaboration could aid students' meaning-making process of chemical terms.

Teacher-centred learning, where teachers typically do most of the talking, is unlikely to result in students' engagement in using chemical language (Bleicher et al., 2003). Questions from teachers are usually not to probe students' understanding but to elicit correct answers. The iVR learning task could include open questions to engage students in using chemical language to construct conceptual explanations. From students' elaborations, teachers and their peers could better monitor whether students use chemical terms appropriately and then provide feedback. The cycle of being critical of each other's scientific explanations could propel students' scientific understanding (Repice et al., 2016). Scientific terms could be introduced to students after using their everyday language to articulate their understanding and help students better retain and apply them (Brown et al., 2010). For example, specific terms (*e.g., homogenous mixtures*) could be introduced after students explained what a solution is using their own words (e.g., "It's even all the way throughout and parts of it are equal like you can't tell the difference between like there is salt and water, and it just looks like water.") (Song & Carheden, 2014).

An iVR experience can be complex and ill-defined to promote collaboration between students (Care et al., 2015). Students tend to work alone when facing a task that they perceive as simple, but they are more likely to ask for help from someone when the task becomes complicated (Wismath & Orr, 2015). The challenging task can stimulate students to share their knowledge and come up with a strategy to solve the task. However, challenging tasks did not always result in students' collaboration and development of knowledge. The lack of ability to function as a group can inhibit students' collaboration (Webb, 2013). For example, students' failure to voice their ideas or listen to others could result in ineffective group work (Barron, 2003).

Open questions could be incorporated into the iVR learning experience to prompt students' engagement in scientific discussion. However, presenting open questions to a group of students does not necessarily lead to productive collaborative discussions (Nokes-Malach et al., 2015). The iVR task can be organised to follow a Predict - Observe - Explain (POE) strategy. The POE strategy, stemming from the constructivist principle of scaffolding, has been used to help students focus on their prior knowledge and take it further (Kearney et al., 2001). By telling students to engage with their prior knowledge, they would have an agency to pick and test the ideas that are meaningful to them (Hennessy et al., 2007). For example, when students were explicitly prompted to observe visualisation, experiment with it, and critique each other's results, they were more successful in integrating various concepts to justify their experiment results. In contrast, students who simply observe the chemistry visualisation tend to miss the link between macroscopic and submicroscopic phenomena (Chang & Linn, 2013).

2.4 Hydrogen Bonding and Snowflake Formation

Intermolecular forces, such as hydrogen bonding, are fundamental chemistry concepts essential to explain various natural phenomena, such as phase changes, solubility, and molecular structures. Despite its significance, students often harbour various alternative conceptions of hydrogen bonding, leading to challenges in predicting the boiling points of compounds (Schmidt et al., 2009; Henderleiter et al., 2001) and the physical properties of materials (Cooper et al., 2012). Common alternative conceptions of hydrogen bonding include confusion between intramolecular bonds and intermolecular forces and mistakenly believing that intramolecular forces are weaker than intermolecular forces (Nicoll, 2001). Students also tend to resort to rote memorisation of hydrogen bonding as a bond between hydrogen atoms and nitrogen, oxygen, or fluorine atoms (Levy Nahum et al., 2010; Ünal et al., 2006).

The topic of hydrogen bonding was typically taught in the context of boiling points (Glazier et al., 2010; Kararo et al., 2019). While they investigated students' understanding of the interaction aspect of hydrogen bonding (e.g., type of bond, bond strength), the 3D structural aspect, such as the directionality of hydrogen bonding, remains unexplored. Understanding the 3D aspect is crucial, given its role in explaining various physical properties of materials, including the unique properties of water (Brini et al., 2017). For instance, recognising the tetrahedral organisation of hydrogen bonding in water elucidates why ice floats on water – a notable anomaly of water (Housecroft, 2020).

The formation of snowflakes could be used as the context for learning and applying the concept of hydrogen bonding in water molecules. Advanced chemistry understanding of concepts such as thermodynamics was needed to explain the crystal formation of snowflakes. Despite the complexity involved, undergraduate students possess sufficient knowledge to explain the hexagonal, six-fold symmetry of snowflakes in connection to hydrogen bonding among water molecules and hydrogen bonding in tetrahedral structures among water molecules (Housecroft, 2020). Although focusing on one or two molecules enables students to learn the characteristics of hydrogen bonding, understanding natural phenomena, like snowflake formation, demands an explanation of interactions among numerous water molecules (Talanquer, 2011).

2.5 Summary

Immersive virtual reality (iVR) can potentially improve student's learning experiences. With the aid of the increasingly more affordable head-mounted display (HMD), more students can experience being transported into another virtual environment. Unlike other media, iVR can evoke a unique sense of "being there" or physical presence. It was assumed that students' learning outcomes would be positively affected by the increase in presence in the learning environment. With the goal of improving students' learning engagement and performance, many researchers investigated the educational benefits of iVR.

Table 2.1

Ways to Evaluate iVR Learning Benefits and Limitations in Response to the Research Gaps

Gaps in the previous evaluation of educational iVR	Possible approaches in evaluating iVR for chemistry
Limited evaluation of declarative knowledge beyond information recall.	Evaluate students' scientific understanding from student-generated representation (e.g., diagrams, verbal, gestures) – *Section 2.2.1.*
Limited studies evaluated how students use iVR to learn.	Evaluate students' interactions during the iVR learning activity – *Section 2.2.2.*
Limited studies performed in-depth analysis of students' perceptions through semi-structured interviews.	Evaluate students' perceptions via semi-structured interviews. Consider using a theoretical framework to inform the inductive interview analysis – *Section 2.2.3.*

Educational benefits of iVR were generally evaluated through students' learning performance after iVR or their perceptions of their iVR experience. For learning performance, most studies evaluated it through pre/post questions that consist of short-answer or single-tier multiple-choice. A deeper understanding of students' level of knowledge can be achieved by evaluating student-drawn diagrams, verbal explanations, and gestures. Previous iVR studies rarely reported how the students achieved or did not achieve the learning objective. A closer look at students' interactions during the iVR activity could better inform how students use iVR to assist their learning. For students' perceptions, the self-reported Likert scale was commonly used, while a limited number of studies used semi-structured interviews or written self-reflection. Studies in computer-supported learning suggest that adopting a theoretical framework to guide the inductive analysis of students' perceptions could unravel more insight into students' different approaches to learning with the medium. The summary of research gaps in terms of the evaluation of educational benefits of iVR and possible ways to address them are presented in Table 2.1.

Table 2.2

Strategies for Addressing Research Gaps and Challenges in Learning Chemistry Through iVR

Gaps in the previous iVR studies for chemistry	Challenges in learning chemistry	Possible approaches for chemistry iVR-based activity
Limited studies allowed the exploration of many molecules or complex molecules in iVR.	Difficulty in predicting emerging chemical properties due to abstract chemical entities.	Visualising and intuitively interacting with complex molecules– *Section 2.3.1.*
Limited studies considered and implemented specific learning approaches in the iVR learning tasks.	Typical piecemeal presentation of chemistry topics makes it difficult for students to link the topics.	Constructivist learning approaches can help students contextualise chemistry ideas to explain natural phenomena – *Section 2.3.2.*
Limited studies implemented collaboration in the iVR learning tasks.	Students are unfamiliar with complex chemistry languages and often resort to rote memorisation.	Making chemistry language meaningful through social interactions between students – *Section 2.3.3.*

iVR has great potential to assist students in learning chemistry. Students have faced challenges in learning chemistry, including the abstract nature of chemical entities, the piecemeal delivery of chemistry concepts, and the complex chemistry language. Various approaches could be considered to address those challenges in iVR. Students could create a concrete understanding of chemical systems by visualising and interacting with 3D molecular structures in iVR. Previous iVR studies for chemistry generally allow students to observe simple 3D molecular structures. In relation to developing comprehensive scientific explanations, students could be situated in a complex real-life problem in iVR to help them link various chemistry concepts. Yet, most iVR chemistry applications include linear storylines (e.g., following laboratory protocol) or few observation tasks. Finally, students could use chemistry ideas and terms more meaningfully by sharing the iVR environment with other students. Although collaborative iVR has been explored in other fields, like geography, it was still limited to chemistry education studies. The summary of previous iVR studies, challenges in chemistry learning, and possible approaches to address the research gaps is presented in Table 2.2.

Chapter 3. Research Methods

This chapter presents the research design for evaluating students' interactions, conceptual changes, and perceptions of their experience within an iVR environment in comparison to magnetic models. The context of this study, including the research questions, participants, and data collection procedures, is described. The details of the learning activity with magnetic models and iVR, including the prompts, are presented. Furthermore, the data analysis methods and the research rigours considerations are addressed in this chapter as well.

3.1 Research Design

The aim of this study is to understand the educational benefits of iVR for learning the concepts of hydrogen bonding and snowflake formation. In the educational context, students' perceptions of learning environments can influence their interaction within the environment and eventually impact their learning outcomes (Struyven et al., 2005). Therefore, rather than simply collecting pre- and post-tests of the intervention, an in-depth analysis of learners' perceptions and interaction within the IVR environment is required to determine the benefits of IVR for learning.

Qualitative research methodology (Creswell & Poth, 2017) was deemed appropriate for addressing the aim of this study. By conducting a qualitative study, it was possible to make meaning from students' actions and perceptions of each learning medium. The close-up look at the participants' experience helped to answer "why" and "how" questions (Merriam & Tisdell, 2009). For example, "How do students learn with iVR?". In contrast, quantitative studies could limit the complexity of students' experiences to predetermined hypotheses or categories (Patton, 2002). Instead of testing a certain theory or measuring the impact of the learning medium, the researcher was interested in inductively identifying processes and reasons why certain learning mediums are beneficial or not beneficial. Thus, a qualitative research methodology was chosen.

A case study research design (Merriam & Tisdell, 2009) was adopted in this study. With this research design, I investigated the educational benefits of iVR through an exploration of a bounded system, a case. In this study, a case was conceptualised as a pair of students (Merriam & Tisdell, 2009). Due to the unique 3D visualisation and interactivity of iVR, students may use different ways to approach the learning content and express their ideas (Matovu et al., 2022; Won et al., 2019). Therefore, for each case, inductive multimodal analysis (Jewitt, 2013) was conducted to capture the possible complexity of students' learning experiences with iVR. Inductive multimodal analysis was particularly appropriate for deriving meaning from students' interaction with digital media because digital media potentially supports new ways of communication and, hence, new ways of sense-making (Jewitt, 2013). The inductive multimodal analysis involves a detailed description of how the participants use more than languages – gaze, gestures, and body movements – to interact with the media and other people.

A cross-case analysis was adopted to strengthen the validity and stability of the result from a single case (Merriam & Tisdell, 2009). The thematic analysis across cases, or cross-case analysis, involves collecting and analysing the similarities and differences in data from multiple cases to answer a particular research question (Miles & Huberman, 1994). The inductive and iterative process was finalised by an interpretive phase to report the meaning of the cross-case analysis (Creswell & Poth, 2017), which, in this study, is related to the education benefits of iVR.

This research investigates students' learning interactions, outcomes, and perceptions of their experience of immersive virtual learning (iVR) in comparison with magnetic models for learning chemistry. The chemistry concept we are focusing on is hydrogen bonding between water molecules in relation to the formation of snowflakes. The overarching question of this study is: "What are the educational potentials of immersive virtual reality (iVR) for first-year students' chemistry learning compared to magnetic models?". The research questions guiding this study are as follows:

Research Question 1. Concerning students' learning interactions and conceptual changes:

(a) How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions when using *magnetic models*?

(b) How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions within an *immersive virtual reality* environment?

Research Question 2. Concerning students' perceptions of their experience:

(a) How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation when using *magnetic models*?

(b) How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation within an *immersive virtual reality* environment?

Qualitative research approaches using inductive multimodal analysis and cross-case analysis were adopted in this study to analyse students' learning interactions and perceptions. The details of the research design taken in this study to address each research question are presented in Table 3.1.

Table 3.1

Research Design: Research Gaps, Research Questions, Data Collection, and Data Analysis

Research gaps identified from literature review	Research questions	Data collection	Data analysis	Quality standards	Results
Limited evaluation of knowledge beyond information recall – *Section 2.2.1* Limited evaluation of students' use of iVR – *Section 2.2.2*	Students' interactions and conceptual changes with magnetic models and iVR (RQ. 1).	Student-generated drawings and explanations (Pre/post-tests). Videos of students' interactions with magnetic models and iVR.	Inductive multimodal analysis of students' diagrams and explanations. Cross-case analysis of multimodal data.	Data triangulation, interrater, personal bias check, audit trail, mitigating ethical concern.	Chapter 4
Limited studies performed in-depth analysis of students' perceptions – *Section 2.2.3*	Students' perceptions of their experience with magnetic models and within an iVR environment (RQ. 2).	Semi-structured post-magnetic models and post-iVR interviews.	Cross-case thematic analysis of students' interviews.	Data triangulation, interrater, personal bias check, audit trail, mitigating ethical concern.	Chapter 5

3.2 Participants

Participants were recruited from first-year chemistry classes at an Australian University. Students from this cohort did not necessarily take chemistry subjects in high school or major in chemistry at university. They took the first-year chemistry class as a requirement for their majors, which include environmental science (marine science), pharmacy, health science (advanced biomedical, laboratory medicine), chemical engineering, food science, and nutrition.

Forty students (16 females and 24 males) volunteered and were paired up depending on students' availability to come to the learning session during the semester. Students choose when they want to participate in the study via an online scheduling platform (doodle.com). The learning session was conducted in Semester 1 of 2021 (March – May). Students received an extra 5 points towards their final scores for participating in this study.

3.3 Data Collection

All students went through the learning sessions in pairs. The learning activities include the exploration of hydrogen bonding in the context of snowflakes with magnetic models and within an iVR environment. Ethics approval (HRE2020-0081) was obtained from the University's Research Ethics Committee. In each learning session, a pair of students signed the consent form and completed the activity with magnetic models, followed by an iVR activity. The learning session comprised of the following:

1) Magnetic model: pre-interview (15-25 minutes), activity with magnetic models (7-20 minutes), and post-interview (15-25 minutes).
2) iVR: pre-interview (15-25 minutes), an activity within iVR space (30-70 minutes) and a post-interview (15-25 minutes).

Semi-structured interviews were performed before and after each activity to investigate students' learning and perceptions of the magnetic models and iVR learning activity. Students' interactions during pre/post-interviews and during each learning activity were audio and video recorded. In addition to audio and video recordings of the room where the learning activities took place, students' views of the virtual reality space were video recorded. Conversations that took place during the learning activities and interviews were transcribed verbatim.

3.4 Interview Prompts

The interview consisted of two main parts: students' learning (pre/post-tests) and students' perceptions of the iVR learning experience. The researchers acted as interviewers instead of as tutors or teachers. As an interviewer, the researcher aimed to guide the students in progressing through the interviews, including the pre/post-tests, without giving students the correct answers.

3.4.1 Interview - Students' Conceptual Understanding

Students were given a picture of magnified snowflakes to assess how students conceptualise hydrogen bonding in the context of snowflakes (Figure 3.1). Students were asked about what they noticed about the snowflakes and how the water molecules interact to form a snowflake.

Figure 3.1

Picture of Real Magnified Snowflakes

To better understand students' conceptual understanding of hydrogen bonding, students were asked to draw a diagram of interactions of water molecules using paper and pencil. While they were drawing, they had to provide verbal (sometimes gestural) explanations of their drawing. The interviewer gave the prompt verbally. The list of interview questions is shown in Table 3.2.

Table 3.2

Interview Prompts: Students' Learning Before and After Each Learning Medium

Segments		Prompts
Pre-interview	Snowflakes	Look at the picture of magnified snowflakes. What do you notice about the shape of snowflakes? How do you explain the shape of snowflakes?
	Drawing	Please draw a water molecule at the centre of the paper. Picture this molecule existing at a significantly low temperature, almost 0° C. Please draw another water molecule interacting with the first water molecule you have drawn. Why did you draw the water molecule in that way? Next, another water molecule comes close to the first one. How would you draw the interaction between those water molecules? (This prompt was reiterated until students conveyed that additional water molecules could not interact with the first one.)
Post-interview	Drawing	Do you want to change your drawing? What kind of change did you make in your drawing? Why did you make those changes?
	Snowflakes	At this point, do you see any connection between what you have learned so far with snowflakes? If yes, how do you see the link between the concepts you learned and snowflakes?

3.4.2 Interview - Students' Perceptions of Learning Experience

To gain a better view of students' perceptions of their conceptual changes and their experience with IVR, a series of questions were asked in a semi-structured manner. The main questions asked in the semi-structured interview before and after each learning media are shown in Table 3.3.

Table 3.3

Interview Prompts: Students' Perceptions

Topic	Questions
Learning	What did you learn or reinforce after going through magnetic models/ iVR learning activities?
Overall experience	How was the experience with magnetic models/ within iVR? What would you change if you were designing a learning activity with magnetic models/ within iVR?
Collaborations	How easy/difficult was it to collaborate with your partner during the activities with magnetic models/ within iVR? How did working with your peers impact your learning?
Comparisons of learning media	How does this compare to other learning media? Which learning activities help you form your current understanding of hydrogen bonding within snowflakes? Why?

3.5 Learning Activities

This study used two learning media: (1) magnetic models and (2) immersive virtual reality. A team of chemistry experts, educational researchers, and doctoral students met in a series of meetings to define the main learning goals for each activity in consideration of first-year chemistry curriculum guidelines. All media covered similar learning goals on the water molecules' intermolecular interaction and structures in relation to the six-fold symmetry of snowflakes. Four main aspects were identified: molecular interactions, simple molecular structures, complex molecular structures, and snowflakes' formation. Each aspect is then further specified into smaller learning goals, such as *optimal angle* or *optimal distance*. The overview of learning goals covered in this study is shown in Table 3.4.

Table 3.4

Main Learning Goals

Concepts		Descriptions
Molecular interactions	Attraction and repulsion	Hydrogen bonding forms between an oxygen atom of one water molecule and a hydrogen atom of another water molecule.
	Intermolecular vs. intramolecular bond.	The hydrogen bond is between water molecules, and it is weaker than the covalent bond.
	Electron density	The O-atom is electron-rich, and the H-atoms are electron-poor regions.
	Optimal distance and angle	When water molecules interact at optimal distances and angles, they create strong hydrogen bonding.
Molecular structures (simple)	Tetrahedral	One water molecule can form up to four hydrogen bonding and are arranged tetrahedrally.
	Hexagonal	When multiple water molecules form hydrogen bonding, they form a stable hexagonal shape.
Molecular structures (complex)	Ice lattice: hexagonal channel	An ice lattice has hexagonal patterns or channels when viewed from multiple angles.
	Ice lattice: tetrahedral subunit	An ice lattice has a tetrahedral subunit when viewed from multiple angles.
Snowflakes' formation	Scale	Molecular structures are so much smaller than snowflakes.
	3D growth	With an increasing amount of water molecules, molecular structures grow into snowflakes in a 3D direction.

3.5.1 Magnetic Models

The magnetic model (WaterKit®) represents water molecules, featuring one oxygen atom (shown as red) and two hydrogen atoms (shown as white). The surface of the magnetic models has four magnetic sites—two on each hydrogen atom and two on the oxygen atom (Figure 3.2). Magnetic interaction occurs between the sites, with hydrogen attracting the oxygen of another water molecule while repulsing the same atoms (e.g., hydrogen repels hydrogen on another water molecule). The magnetic forces metaphorically depict electrostatic attraction between electron-rich and electron-poor areas. Due to the complexity of forming a massive uniform ice lattice, a sufficient number of magnetic models were provided to create a simplified 3D ice lattice.

Figure 3.2

Two Magnetic Models of Water Molecules

Seated in front of the interviewer (Figure 3.3), students received verbal prompts after the pre-interview. Each student was initially provided with two magnetic models and, later, five more. Students were given a maximum of 25 magnetic models if they requested more. Students were prompted to discuss their observations with their peers during the activity. The prompts used during the magnetic model activity are detailed in Table 3.5. The activity was concluded with a post-interview when the pair of students were satisfied with their exploration of magnetic models.

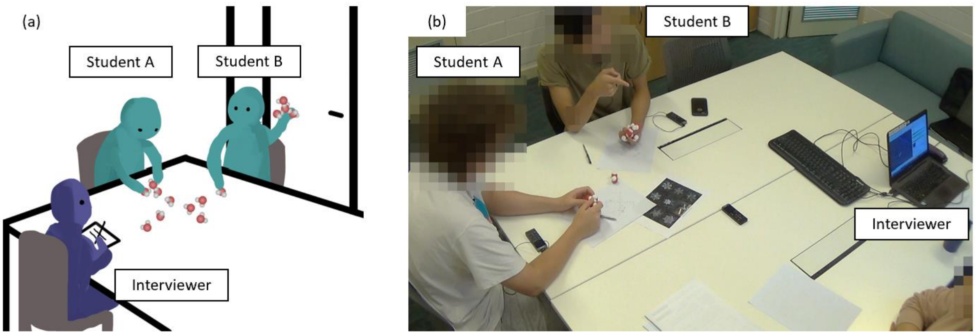
Table 3.5

List of Prompts in the Activity With Magnetic Models

Segments		Prompts
Magnetic models	Two magnetic models	These are models of water molecules. They were designed to learn the characteristics of water molecules. Explore it and let your partner know what you have found. What do you notice? Why do you think that could happen? Put the models on the table. Try to detach two water molecules. What do you notice? Why?
	Seven magnetic models	What do you notice? Why do you think that could happen? How about testing your hypothesis about the maximum number of water molecules that can attach to a water molecule? Why xx number of water molecules? Is it a stable structure?

Figure 3.3

Arrangement in a Learning Activity with Magnetic Models



Note. (a) Reconstruction of typical spatial arrangement during the magnetic model activity, (b) screenshot of one of the sessions.

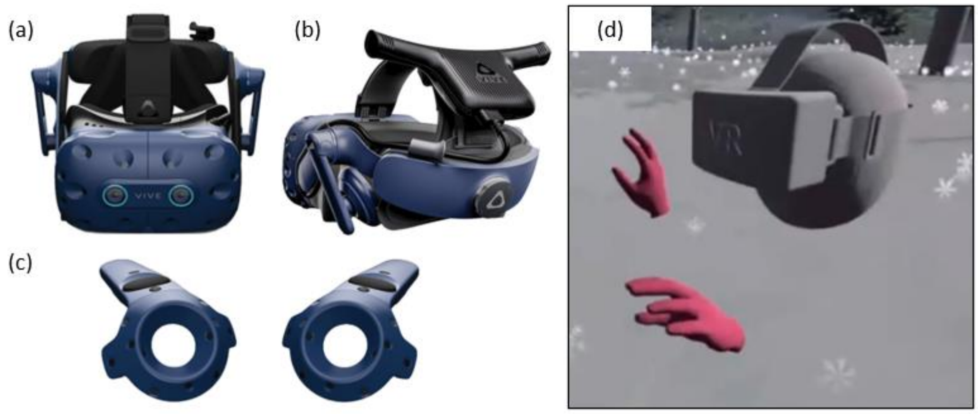
3.5.2 Immersive Virtual Reality (iVR)

Each student wore an HTC-VIVE Pro Eye VR headset with wireless adapters and two controllers (Figure 3.4). They shared a 3 m x 3 m space. Before students wore the headsets, students were given a short introduction about how to interact with each other and with the objects inside the virtual environment. The researchers also explained safety precautions before the iVR learning activity. The details of the pre-iVR activity instruction are presented in Appendix A. The researchers observed the students from outside the boundaries. The student's views of the IVR space were cast into two big monitors so the researcher could also monitor what students saw in real time. Inside the virtual space, each student was represented as an avatar of floating headsets and a pair of pink hands (Figure 3.4d). Therefore, students could see and hear each other.

With iVR, students transcended physical and virtual space. Their virtual self, avatars, moved the molecules in the virtual space as if they were real objects moving in real physical space (Figure 3.5). Unlike magnetic models, the models of water molecules in iVR were bigger in size and number, and they were floating in the air. Using the controllers, students could use their hands to interact with the 3D objects inside the virtual space. Students could also walk around to explore the virtual space.

Figure 3.4

HTC-VIVE Pro Eye iVR Headset and Avatar



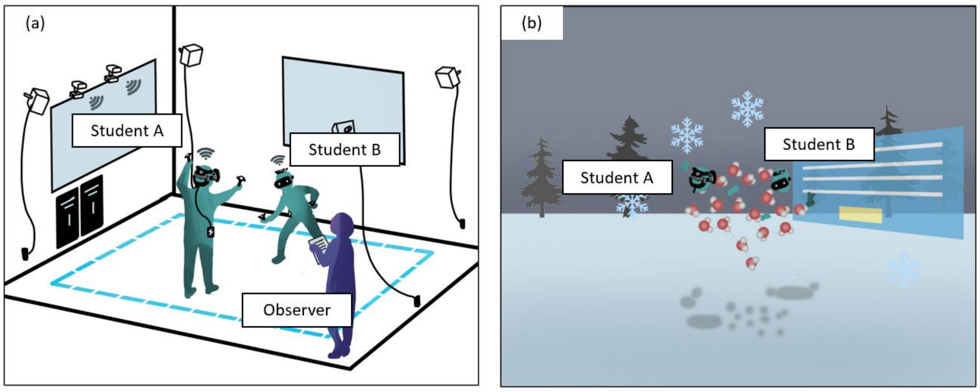
Note. (a) Front view of the headset, (b) back view of the headset showing the wireless adapter attached, and (c) left and right controllers (VIVE, 2023), (d) avatars.

The iVR learning activity was designed to explore the gradual growth of ice crystals or snowflakes (Figure 3.6). When students entered the iVR space, they were welcomed by a scene of a winter forest to familiarise themselves with iVR functionalities. After the winter forest scene, the activity starts by connecting two water molecules, five water molecules (tetrahedral shape), a single layer of ice, three layers of ice, and finally, the comparison of ice lattice and snowflakes.

After the task of comparing ice lattice and snowflakes, a video was played on the screen inside the iVR space. The video showed and explained how environmental factors influence the symmetry and the unique branches of snowflakes. Then, students were transported back to the winter forest to wrap up the experience.

Figure 3.5

Physical and Virtual Spaces During the IVR Learning Activity

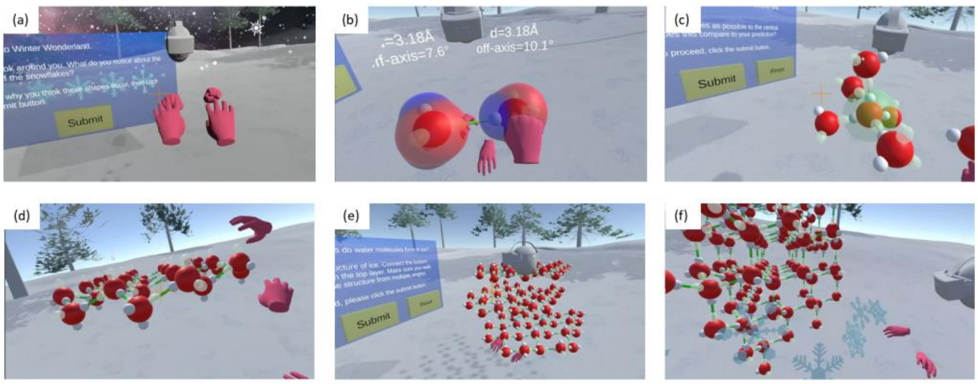


Note. (a) Reconstructed view of the room setup – what the observers were seeing, (b) reconstructed view of the virtual space – what the students were seeing.

In each step of the IVR learning activity, students were given a prompt to build a structure, observe, and discuss it with their partner. The prompts were split into three smaller steps (predict-build - explain) following the POE models (Treagust et al., 2014) to scaffold students' exploration and conceptual understanding. Further details about the prompts conducted in this study can be found in Appendix A.

Figure 3.6

Screenshots of Main Tasks in the iVR Learning Activity



Note. The order of IVR learning tasks: (a) winter forest, (b) creating a hydrogen bond between two water molecules, (c) creating tetrahedral, (d) creating a single layer of ice, (e) connecting three layers of ice, and (f) comparing ice lattice with snowflakes.

3.6 Data Analysis

A total of 63 hours of learning session audio and videos, 119 student-generated diagrams, and 20 sets of log data were recorded. Inductive multimodal analysis (Jewitt, 2013) and cross-case analysis (Creswell & Poth, 2017) were adopted to qualitatively analyse the data for emerging patterns of students' interactions and categories of students' conceptual changes and perceptions.

3.6.1 Analysis of Changes in Students' Conceptual Understanding

For this study, the analysis of six cases or pairs of students was presented. We required the student-generated diagram and their snowflakes' explanation to better understand students' conceptual understanding before and after each learning mode. However, participants did not always consent to provide a drawing after each learning activity because they felt they could not draw or their ideas were impossible to draw. Only six pairs completed all the student-generated diagrams after each learning activity. Therefore, we focused on these six pairs: Mark-Ana, Elena-Fiona, Nigel-Jasper, Kenan-Pascal, Tiana-Renee, and Zeke-Turner. These names are pseudonyms.

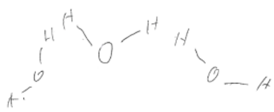
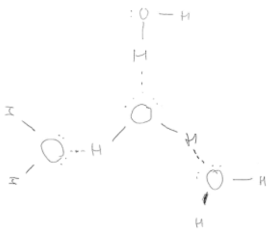
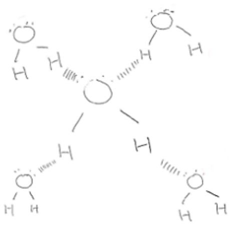
Students' learning, as depicted in their diagrams, gestures, and verbal explanations, was categorised to discern the changes in their understanding following the magnetic model and iVR learning activities. The coding schemes for categorising students' understanding of hydrogen bonding and snowflakes' formation were adapted from Matovu et al. (2023b).

For the concept of hydrogen bonding, students' understanding of the hydrogen bonding between water molecules was categorised into four categories (Table 3.6). Based on their drawings and explanation, students' understanding ranged from an unclear understanding of hydrogen bonding (Category A), an unclear understanding of the role of lone pairs (Category B). a clear understanding of hydrogen bonding on a 2D plane (Category C), and an unclear understanding of hydrogen bonding on a 3D plane (Category D). The coding for this categorisation underwent verification and validation by two other researchers, ensuring agreement on the categorisation of all students.

For the concept of snowflake formation, the different combinations of ideas about molecular structures and their dimension resulted in several categories of students' explanations of snowflake formation. Students' explanations of snowflakes involved ideas about molecular structures such as hydrogen bonding, hexagonal symmetry, and tetrahedral subunits. The dimension of the molecular structures was explained by students as an interaction of water molecules in a 2D plane (flat) or in a 3D plane. See Appendix B (Table B.1) for the detailed coding scheme of students' explanations.

Table 3.6

Coding Schemes for Students' Understanding of Hydrogen Bonding

Category	Description	Example of student-generated diagram	Example of student's verbal explanations
A – Unclear understanding of hydrogen bonding	Hydrogen bonding as H-H bonds or do not recognise the difference between intermolecular and intramolecular forces.		*"They're close to each other, but they're not actually ... Unless you add something (dust particles) to it, and then you get hydrogen bonding."*
B – Unclear understanding of the role of lone pairs	Hydrogen bonding as an attraction between oxygen and hydrogen of another water molecule. However, not sure about lone pairs and the number of water molecules attracted to a water molecule.		*"Because because it's a polar, yeah. Because the oxygen is highly negative. And then the hydrogen would be, like, not as negative."*
C – Clear understanding of hydrogen bonding on a 2D plane.	Hydrogen bonding as an attraction between oxygen and hydrogen of another water molecule. Each lone pair of O atoms is capable of attracting another water molecule.		*"So there's one they're attached to, there is another one attached to the lone pair that has been attached to lone pair, and that oxygen attaches the hydrogen. The dotted ones are intermolecular forces."*
D – Clear understanding of hydrogen bonding on a 3D plane.	Hydrogen bonding is an attraction between oxygen and hydrogen atoms of other water molecules. The maximum number of water molecules attracted to a water molecule is *four,* forming a tetrahedral (3D).		*"Yeah, the oxygen and hydrogen that are coming out of the plane and the dash going back into the plane. There's probably to do with the intermolecular forces and electronegativity forcing them away."*

3.6.2 Analysis of Students' Interactions

Video recordings of students' interactions during the magnetic model and iVR activity were prepared prior to analysis. For iVR, further video preparation was necessary to get a synchronised view of the pairs and the researcher by creating a composite video. For each pair of students, a composite video was generated by synchronising the audio and videos of the iVR learning session that comprised of (1) *top – a* room view, (2) *bottom left* – a student's view of the iVR space, and (3) *bottom right* – the peer's view of the iVR space (Figure 3.7).

The researcher team members reviewed several videos of the students' interaction during the magnetic model and iVR activity to identify general patterns of students' interactions and conceptual discussion. Three videos were further inductively analysed (Patton, 2002) to determine the coding scheme. Time-stamped transcripts of student conversations and actions during both learning activities were created to facilitate the coding process. Additional rounds of multimodal analysis (Jewitt, 2013) were conducted to create a detailed description of each pair of students. Each pair contains a description of the conceptual, social, and spatial aspects. Spatial, social, and conceptual interactions of six pairs were constantly compared using cross-case analysis (Creswell & Poth, 2017) to identify emerging patterns of interaction. Emerging patterns of students' interactions were discussed and checked with the doctoral supervisors until an agreement was reached.

Figure 3.7

A Synchronised Video of Interactions Between Students A and B

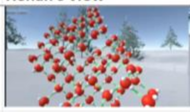
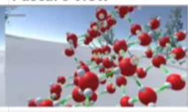
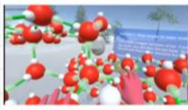
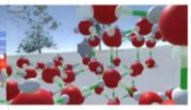
Note. Videos of the real space/ room (top), student A's view of the iVR space (bottom left), and student B's view of the iVR space (bottom right).

Spatial Aspect. Students' movements during magnetic model activity and inside the iVR space were analysed in relation to their conceptual discussion. For magnetic models, students' movements pertinent to conceptual discussion involved (a) pushing and retracting two magnetic models and (b) constructing linear, tetrahedral rings (pentagons, hexagons, and heptagons) and 3D lattice structures. The duration of time students spent on each action was documented in the time-stamped transcripts.

For each task, students' actions and the 3D structures that became the object of students' actions were recorded. An example of a description of spatial exploration of a student in iVR is as follows: "Student A walked around an ice lattice to observe it from different angles and notice the hexagonal channels". Such a description is added alongside the transcript and a screenshot of the composite video (Figure 3.8).

Figure 3.8

Time-Stamped Transcripts of Students' Discussions in the iVR Learning Activity

	Timespan	Speaker	Conversation	Kenan's view	Pascal's view	Room's view
187	24:38.0 - 24:45.0	Kenan	Okay. so what do we got going on? It's kind of hard to describe. It's like a...			
188	24:47.0 - 24:48.0	Pascal	just endless hexagons.	Kenan rotates the ice lattice to view from different angle.	Pascal observes the ice lattice as Kenan rotates it.	
189	24:49.0 - 24:57.0	Kenan	Yeah. I'm trying to hold it in a way like this. So you can kind of see the layers. .			
190	24:57.0 -	Pascal	I'm inside the honeycomb.			
191	25:01.0 -	Kenan	So if you're looking at one of these central water things,			
192	25:04.0 -	Pascal	Yeah			
193	25:06.0 - 25:23.0	Kenan	it's all.. so each of these three ones here, these three, the bonds coming off all vertical. It's like kinda, yeah makes sense. It's all vertical, hexagons are vert..okay..	Kenan walk into the ice lattice and points at tetrahderal subunit.	Pascal is inside the ice lattice.	

Social Aspect. Students' verbal interactions, including asking questions, reiterating, providing short responses, or elaborating on ideas, and the recipients of their responses (peers or the interviewer) were documented. During the iVR activity, the researchers were not present inside the virtual space; thus, no/minimal interactions were recorded. The way students used the space (sharing the 3D molecular structures or not) was also recorded.

Conceptual Aspect. For each task, the concepts discussed by pairs of students were recorded and matched to the intended learning goals (Table 3.4). For magnetic models, three concepts were identified: attraction-repulsion, tetrahedral structure, and hexagonal structure. For iVR, the discussion can be categorised in relation to *simple* and *complex structure tasks* because students exhibited distinctive discussion and behaviour during these two tasks. The concepts identified for the simple structure tasks (two water molecules, tetrahedral tasks) included features of water molecules, the formation of hydrogen bonding, the relation of bond strength with angle and distance, and tetrahedral. The concepts identified for the complex structure tasks (single layer, ice lattice tasks) were hexagons, tetrahedral subunits, snowflakes' formation, scale, growth, and randomness. The level of discussion concerning each chemistry concept was recorded.

3.6.3 Analysis of Students' Perceptions of Learning Experiences

For the analysis of students' evaluation, 20 pairs (students who gave consent) are presented in this study. Students' interviews after the magnetic models and iVR learning activity were transcribed and coded for analysis to understand how they perceived their learning with iVR. Three main categories emerged from the initial inductive thematic analysis (Braun & Clarke, 2006): *visualisation, interactivity,* and *collaboration/communication*. Categories were then created for each theme based on the initial reading of the transcript (inductive) and the known magnetic models and iVR features based on the literature review (deductive). Another theme, *narrative,* was identified in relation to the data and the literature about immersion features (Dede et al., 2017). Two researchers coded the six pairs of students and met to amend the coding schemes and the coding result until an agreement was reached. The author then coded the rest of the pairs. The coding result and emerging pattern were discussed with doctoral supervisors until an agreement was reached. Further refinement of the coding schemes resulted in four main themes of each learning medium:

Theme 1: Visualisation and Theme 2: Interactivity. The visualisation and interaction categories were further specified to understand how students interact and what kind of visuals were highlighted by students. For magnetic models, the visualisation aspect was specified to *1-2 molecules* and *> five molecules* for magnetic models, while for iVR, were *environment*, *simple structures* (i.e., two water molecules and tetrahedral), and *complex structures* (i.e., a single layer of ice and ice lattice). The interactivity aspect was specified to *observe* and *construct* for both magnetic models and iVR. Another mode of interactivity, *play*, was identified for iVR. *Play* refers to picking up and rotating the molecules without the means of connecting them to construct a bigger structure.

A category in this theme was a combination of visualisation and interaction aspects. For example, the category *observes simple structures in iVR* included students who evaluated iVR as a medium that allowed them to be in a different place where they could observe two water molecules (without playing with them). The detailed coding scheme for visualisation and interactivity is included in Table C.1 and C.2 in Appendix C.

Theme 3: Narrative. The content about hydrogen bonding and the shape of snowflakes was designed following the POE models (predict - observe/build - explain) (Treagust et al., 2014) for each learning activity. The narrative theme included students' evaluation of their experience in relation to the task design. Three main categories emerged from students' comments: *test hypotheses, problem-solving,* and *stepwise tasks.* The test hypotheses category included students' appreciation of having the opportunity to apply their prior knowledge to test hypotheses. The problem-solving category included students' comments about improving their analytical skills due to the agency (no intervention) they experienced when solving the tasks in the learning activity. The stepwise tasks category captured students' appreciation of the incremental scaffold they received in their learning activity. Further details about the narrative coding scheme are included in Table C.3 in Appendix C.

Theme 4: Collaboration and Communication. This theme captured students' perceptions of having a partner during the activity with magnetic models and iVR. The collaboration aspect was specified in *group play* and *individual play*. Group play included students who appreciate having a partner for different reasons (bounce ideas, fun, faster). The individual play included students who preferred to complete the activity alone. See Table C.4 in Appendix C for the Collaboration coding scheme.

The communication aspect only applied to iVR because iVR involved a new way of communication compared to traditional classrooms (Bailenson et al., 2004). The communication aspect was specified to *avatar* and *hybrid space*. The avatar category captured students' perceptions of communicating with each other without facial expressions. The hybrid space category included students' perceptions of navigating between real and virtual spaces. See Table C.5 in Appendix C for the Communication coding scheme.

3.7 Research Rigor

The University's Research Ethics Committee granted the ethics approval (HRE2020-0081). All participants signed the participant consent form before participating in the study. Prior to the experiment session, the researcher explained the purpose of the research and told the participant that the learning activity was not a test. Access to the data was restricted to the researcher and the research group. A pseudonym was used in the result and analysis of this study to ensure the participants' anonymity.

The potential risks of using iVR technology include cybersickness (motion sickness) and cognitive burden (Behr et al., 2005). The participants were briefed about the potential side effects and how to depart from the iVR experience safely at any time during the experiment. All learning activities, including the iVR experience, were tested before the session with respect to the potential risks.

Keeping internal validity and reliability is important for the trustworthiness of the result in capturing reality (Golafshani, 2003). Multiple data sources were collected to allow data triangulation in this study (Merriam & Tisdell, 2009). Data were collected by means of student-generated diagrams, audio and video recordings of the learning sessions (learning activity with each medium and the pre/post interviews), and observation notes to confirm the emerging findings. The researcher is aware of the personal bias that may affect the validity of the data (Claire, 2010). As part of the validity procedures, the researcher continuously reflected on these biases: (1) as an instructional designer who prefers iVR technology compared to other media, and (2) as a novice social science researcher with a pure science background. To promote the validity and reliability of the study, multiple members of the research group watched recordings of students' learning sessions and coded the student-generated diagrams and transcripts (Campbell et al., 2013). An *audit trail* detailed record of methods, data, and decision points (such as the changes in the learning activity) was made in the process (Creswell & Miller, 2000).

Chapter 4. Changes in Students' Conceptual Understanding Through a Series of Activities With Magnetic Models and Within Immersive Virtual Reality

This study evaluates students' interactions and conceptual changes when using magnetic models and in an iVR environment. This chapter presented the results of six cases or pairs of students because they completed student-generated diagram tasks before and after the activities with magnetic models and iVR. The focus of the investigation was on hydrogen bonding between water molecules in the context of the formation of snowflakes. This chapter is organised into eight sections.

The overview of students' conceptual changes and interactions is presented in Section 4.1. Sections 4.2 - 4.7 present case studies of six pairs of students with varying levels of prior knowledge, showing their conceptual changes and interactions throughout the activities with magnetic models and iVR. Section 4.8 presents the results of a cross-case analysis of students' conceptual changes and interactions. These sections address Research Question 1.

(a) How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions when using *magnetic models*?

(b) How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions within an *immersive virtual reality* environment?

4.1 Overview

Students have different levels of prior knowledge at the beginning of the learning activity. One pair (Ana – Mark) had an alternative understanding of hydrogen bonding by explaining it as an H-H interaction. Another pair (Elena – Fiona) comprised students with mixed prior knowledge, with Fiona as the one with a slightly better understanding. A third pair (Nigel - Jasper) had a better understanding of hydrogen bonding but was not sure about the role of lone pairs. These student pairs generally were not sure about the formation of snowflakes. Three pairs (Tiana-Renee, Kenan-Pascal, and Zeke - Turner) had a higher prior knowledge by being able to explain hydrogen bonding as an O-H interaction between water molecules and explaining the maximum four hydrogen bonding per water molecule. These pairs with higher prior knowledge generally managed to give some explanation of snowflake formation by focusing on its appearance. The findings showed that these pairs of students exhibited unique patterns of interactions during the activity of magnetic models and iVR, depending on their prior knowledge.

Students with lower prior knowledge showed changes in their conceptual understanding of the O-H interaction between two water molecules. They spent more time and had more discussion during the task that involved two water molecules, trying to learn about how and why O-H attracts while O-O and H-H repels. When they were exposed to more water molecules during magnetic models and iVR activity, these students began to show signs of confusion and resorted to surface descriptions of the complex structure they saw. Their interactions with the water molecules seemed to influence their conceptual understanding. As shown in their diagrams and their verbal explanations, students with lower prior knowledge changed from conceptualising hydrogen bonding as H-H or O-O interactions to O-H interactions after magnetic models and to 3D O-H interactions after iVR. In terms of their explanation of snowflake formation, their explanations shifted from focusing on flat branches after magnetic models to hexagonal symmetry after iVR.

Students with higher prior knowledge showed changes in their conceptual understanding of 3D interaction among many water molecules. Unlike students with lower prior knowledge, these students seemed more engaged during tasks involving many water molecules. During the activity with magnetic models, these students created more complex structures without prompting and were more successful in constructing complex structures during the iVR activity. Due to the limitations of magnetic models, these students focused on the flat appearances of snowflakes and explained the interactions of many water molecules on a 2D plane. Similar to students with lower prior knowledge, these students developed a better understanding of 3D spatial interactions of water molecules after the iVR activity. However, unlike students with lower prior knowledge, these students were able to include more ideas (hexagons, tetrahedral, and scale) in their explanations of snowflakes after iVR.

4.2 Ana and Mark

4.2.1 Conceptual Understanding Before Activities With Magnetic Models

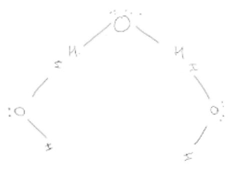
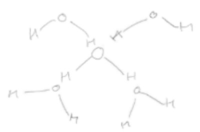
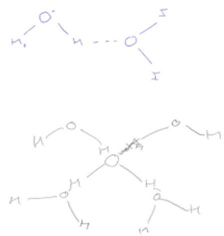
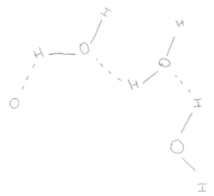
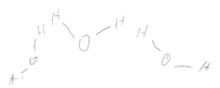
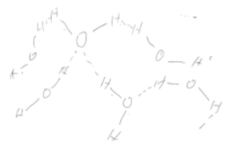
For the concept of hydrogen bonding, Ana and Mark explained that the interaction between water molecules was called hydrogen bonding, but they conceptualised hydrogen bonding as an interaction between hydrogen atoms of different water molecules. Ana drew one or two lone pairs for each oxygen atom.

For the concept of snowflake formation, Ana and Mark noticed that the snowflakes were pretty and symmetrical but were unsure how to explain the snowflakes' formation. Mark focused on remembering some chemistry terms such as "crystal seed" and "crystallisation" without elaborated explanations.

> Mark: *"There's a term for the way these crystals, these crystals occur. […] Just like, Bang. Blocks of crystallization."*

Table 4.1

Change in Ana and Mark's Diagrams of Hydrogen Bonding

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Ana				
	Category A	Category C	Category B	Category B
Mark		[Collaborative drawing with Ana]		
	Category A	Category C	Category A	Cannot be categorised

4.2.2 Interactions With Magnetic Models

Starting with an alternative understanding of hydrogen bonding, Ana and Mark used this activity to learn the nature of hydrogen bonding and the maximum number of hydrogen bonding per water molecule. However, they explained hydrogen bonding and snowflakes' formation by directly describing the observed structure of magnetic models. Their exploration of magnetic models did not help this pair establish why O-H attracts and why snowflakes have a particular symmetry.

Ana and Mark changed their alternative understanding of hydrogen bonding by feeling the attraction and repulsion between two models of water molecules. Initially, both thought that a H atom of a water molecule would "attach" to a H atom of another water molecule. They tested their hypothesis by putting H atoms of two water molecules closer to each other and looked surprised when they felt the repulsion. As explained by Ana:

> Ana: "*I get it now! […] It's going to be [between] hydrogen and oxygen, because [showed attraction with models]. Yeah, while oxygen and oxygen [showed repulsion with models]. Interesting. I need some of these [models].*"

They repeatedly tested each connection (O-H, H-H, and O-O) and felt the attraction or repulsion as the models of water molecules got closer. However, when prompted about the reason for the O-H attraction, Ana and Mark silently looked at each other. Both finally gave short answers by mentioning electronegativity, positive, and negative without further elaboration.

With more models of water molecules, Ana and Mark exhibited similar behaviour of extensive exploration of magnetic models without much conceptual discussion between them. They created chains, cyclic, and tetrahedral structures with their own set of multiple magnetic models. Both were surprised to see that water molecules could form ring structures, similar to the cyclic carbon they saw in class. Because the students were silent after describing the cyclic structure, they were prompted about the stability of the structures. Both then began to shake various structures and talked about a chain being the weakest and a cyclic as the strongest structure in relation to ice crystals. However, neither Ana nor Mark had linked the cyclic structures and the shape of snowflakes during this activity. As elaborated by Ana:

> Ana: *"That [cyclic structure] more stable than a line [chain structure] of the same molecule? […] I guess, if you're trying to form, like if it was wanting to form a crystalline structure or something, you would need rigidity."*

After being prompted, both added as many water molecules as possible to the central water molecules and established that the maximum number of water molecules that can "attach" to a water molecule is four. Apart from describing four binding spots (two on O atoms and one for each H atom), this pair did not further explain why a water molecule could form up to four hydrogen bonding.

Ana and Mark enjoyed extensively manipulating the magnetic models to describe how water molecules interact via O-H attraction to form various structures. However, their limited understanding of hydrogen bonding prevented them from moving beyond what was visually or tactilely represented with magnetic models. They accepted that magnetic models were true copies of water molecules. As shown in their post-interview (Table 4.1), Ana drew water molecules almost touching each other without considering the relative distance between covalent and hydrogen bonding as if copying the models. Ana and Mark's interaction showed that magnetic models helped students challenge their prior understanding of intermolecular attractions, but certain levels of conceptual understanding of relevant concepts were required for students to explain the reason for that molecular interaction.

4.2.3 Conceptual Understanding After Activities With Magnetic Models

For the concept of hydrogen bonding, Ana and Mark's understanding of hydrogen bonding changed from interactions between H-H to O-H of different water molecules. They recognised that water molecules could "attach" with a maximum of four other water molecules. However, the interaction between O-H of different water molecules was represented as close proximity (almost touching), giving the impression that hydrogen bonding is shorter than the covalent bond (O-H within a water molecule).

For the concept of snowflake formation, Ana, looking at their drawing of the tetrahedral, explained that it looked like the branches of snowflakes. Mark added that the structure (branches) would keep growing as more molecules become present. Ana also explained that she might be "just too imaginative" in trying to "fit" their drawing of tetrahedral into the picture of snowflakes in her mind, which indicates that she was still unsure about her explanation of snowflakes. No 3D expansion was mentioned.

4.2.4 Conceptual Understanding Before iVR Activities

For the concept of hydrogen bonding, Ana and Mark explained that the bonds within water molecules differed from the interaction between water molecules. Both represented hydrogen bonding as dashed lines between O and H atoms to show this difference. Both showed a centre water molecule would have four hydrogen bonding. However, Mark simply added several water molecules to his original diagram and represented hydrogen bonding as interactions between O-H and H-H of different water molecules. Ana, in contrast, drew an additional set of water molecules apart from her original diagram. She added positive and negative charge symbols on H and O atoms, respectively, to explain the attraction between water molecules. However, the dashed line for hydrogen bonding was drawn at an odd angle. Ana's diagram suggests that she viewed the whole O atoms as negative without considering the positions and roles of lone pairs. She also might have an alternative preconception of the optimal angle as O-H instead of O-H-O. Compared to their previous drawing, both drew water molecules apart and explained there were optimal distances when water molecules interacted.

For the concept of snowflake formation, both still focused on the flat appearance of snowflakes. Ana did not change her explanation of snowflakes much, apart from repeating that she got a better picture of how water molecules "attach" to form a structure similar to snowflakes. Mark added that it would take "two million" water molecules to form snowflakes, influencing the variety of snowflake branches.

4.2.5 Interaction in iVR

Before the iVR activity, Ana and Mark developed an understanding of O-H intermolecular attraction between different water molecules. However, some ideas, such as the 3D orientation of hydrogen bonding, were still missing. Inside the iVR environment, this pair seemed to engage in more conceptual discussion about the optimum 3D arrangement of water molecules and cyclic formation while exploring simpler structures. In contrast, their interaction with more complex structures resulted in a surface description of the structure with much conviction.

Ana and Mark extensively explored the interaction between two water molecules to apply their knowledge of hydrogen bonding in 3D space. At first, this pair could not form a hydrogen bond because they repeatedly positioned the molecules, almost touching as if they were trying to mimic what they did with magnetic models. Ana, who showed some understanding of distance before iVR activity, pulled the molecules apart to form a hydrogen bond successfully. Mark, who still drew H-H attractions before iVR, tested his idea inside iVR by trying different connections (H-H, O-H, and O-O) and confirmed O-H attractions as hydrogen bonding. From their exploration of two water molecules, they discuss the implication of distance and angle. As Ana explained:

> Ana: *"So strange because they [molecules] want to be at the right distance and the exact right rotation, they're fussy, that's what they are. […] Otherwise, there's no bond or the bond is too weak."*

They concluded that optimal distance and O-H alignment were necessary for a strong hydrogen bond.

Ana and Mark's extensive spatial exploration and discussion of the 3D spatial arrangement of water molecules continued during the tetrahedral task. In iVR, without the presence of the interviewer, both students seemed to have more opportunities to reflect on their prior knowledge. For instance, Mark could not predict the maximum number of hydrogen bonding per water molecule in iVR, which may be caused by his not participating during the previous discussion of tetrahedral with magnetic models. So, in iVR, he tried to connect as many water molecules as possible to one molecule. When hinted about structural growth by Ana, Mark then proceeded to add even more water molecules to the tetrahedral and created pentagons – which seemed to be a surprising finding for this pair. As Mark said*:*

Mark: *"Huh, but they go pentagonal. Interesting. That's cool."*

In the next task, Ana and Mark had no trouble connecting two clusters of water molecules and were excited to see the resulting hexagonal structure.

When seeing even more water molecules, Ana and Mark began to show signs of frustration and demonstrate more of their different perspectives when exploring the structures. For example, while constructing a single layer, Ana has a "zoom-in" perspective by discussing the orientation of lone pairs and H atoms. In contrast, Mark has a "zoom-out" perspective by examining the hexagonal staggered formation. This pair struggled to construct the single layer, perhaps because they tried to divide the labour instead of consolidating their different perspectives to find a joint strategy. Both looked a bit tired during the next ice lattice vs. snowflakes task. When observing the ice lattice, Mark walked around extensively to see the hexagons from different angles while Ana stood still and simply agreed with Mark. Mark tried to reason about the different patterns of snowflakes by explaining the probability effect, while Ana mentioned the variation of angles. However, they seemed unsure how to consolidate their ideas by ending their explanation with comments such as "I have no idea" or "I don't know how I would explain it". As a result, their conceptual discussion did not go beyond surface descriptions of the structures during their exploration of complex structures.

Looking at Ana and Mark's interaction in iVR, they seemed to have the relevant prior knowledge to conceptually engage with simpler structure tasks. As the structures became more complex, this pair seemed to be overwhelmed and focused on the discussion of salient surface features – for Ana, it was the O-H connection; for Mark, it was the ring structures. The different focus can be seen in their post-diagrams (Table 4.1), where Ana drew multiple water molecules hydrogen bonded in a particular orientation, while Mark exhibited more of a zoom-out perspective by drawing staggered hexagons without representation of individual water molecules. However, the interaction with complex structures was still beneficial in relating the 3D hexagonal pattern to the six-fold symmetry of snowflakes.

4.2.6 Conceptual Understanding After iVR Activities

For the concept of hydrogen bonding, both wanted to show the 3D hexagonal formation they saw in the iVR learning activity. Ana explained that the O atoms in her drawing were located on different planes, as she said:

Ana: *"Like the oxygens, [pointing at different O atoms in her drawing] that would be up, that would be lower than that, that would be up."*

Mark did not draw the individual water molecules; therefore, his understanding of hydrogen bonding cannot be fairly identified. Ana still represented hydrogen bonding as dash lines between O and H atoms between water molecules. The angle of O-H interactions in her drawing suggests that Ana did not recognise the role of lone pairs and viewed the whole O atoms as negatively charged.

For the concept of snowflake formation, Ana and Mark explained that water molecules would hydrogen bond into a hexagonal pattern, which is why snowflakes are hexagonal. Both mentioned that the hexagonal structures can form layers to eventually form a 3D ice lattice. They also repeat the explanation about environmental factors concerning snowflakes' symmetry that they heard in the video in iVR.

4.3 Fiona and Elena

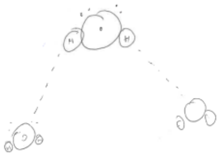
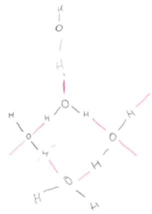
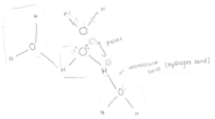
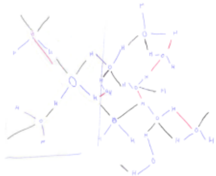
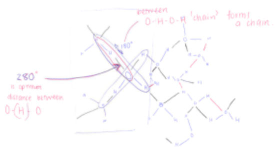
4.3.1 Conceptual Understanding Before Activities With Magnetic Models

For the concept of hydrogen bonding, Fiona and Elena conceptualised the interaction between water molecules differently. Fiona explained that water molecules interacted through hydrogen bonding – an attraction between water molecules – and that it was different from a covalent bond. Fiona recognised that lone pairs of O atoms could attract H atoms of different water molecules. Her drawing also showed that hydrogen bonding is longer than covalent bond. In contrast, Elena showed the interaction of water molecules as an interaction between O-O of different water molecules. After hearing Fiona's explanation, Elena drew lines between O and H atoms of different water molecules and labelled them as intermolecular forces. However, Elena explained that the O-H interaction in her drawing was a functional group (hydroxyl). Elena's explanation suggests that she was still unsure about the difference between inter and intramolecular bonds even though she had heard Fiona's explanation.

For the concept of snowflake formation, apart from describing that a snowflake looked symmetrical and pretty, Fiona and Elena did not know what to say about the formation of snowflakes. When they saw their drawings of chain structures, they wondered how they were related to snowflakes.

Table 4.2

Change in Fiona and Elena's Diagrams of Hydrogen Bonding

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Fiona	 Category B	 Category D	[Made no changes from the previous diagram] Category D	 [Collaborative drawing with Elena] Category D
Elena	 Category A	 Category C	 Category C	 Category D

4.3.2 Interactions With Magnetic Models

Fiona had a better understanding of hydrogen bonding than Elena. During the activity of magnetic models, the structures they created seemed to be a combination of each student's prior knowledge. This resulted in a discussion of various fundamental ideas of hydrogen bonding, such as inter vs. intramolecular bonds and tetrahedral structures. Although they developed a better explanation of hydrogen bonding, this pair has yet to establish the reason for the symmetry of snowflakes.

The interplay between Fiona and Elena's prior knowledge helped this pair to establish the nature of hydrogen bonding using the magnetic models. With limited prior knowledge, Elena found that water molecules interact through O-H attraction by feeling the attraction and repulsion between the magnetic models. Fiona, unsure about the role of lone pairs, confirmed Elena's assertion and added that there were two spots on the oxygen to attract two more water molecules. Elena pondered about Fiona's comment, but because of her limited prior knowledge, Elena could not differentiate between covalent and hydrogen bonding. Using the models, Fiona supported Elena by pointing out which ones were covalent and hydrogen bonding, as shown in the following:

Elena: "*So then, does that mean the oxygens, they can take up to four bonds, right? [Are all four bonds the same?] I feel like that's not. But I don't know."*

Fiona: "*So those are two intermolecular and two intramolecular. […] Because this is covalently bonded hydrogen in the water molecule. But then if oxygen was to bond with like another hydrogen from [another] water molecule here, that wouldn't be an actual like bond. Yeah, more of an interaction.*"

Fiona and Elena continued to manipulate and discuss the structures created using magnetic models in relation to their individual prior knowledge. Fiona made a cyclic structure and immediately noticed its similarity with snowflakes by saying, "Oh, I made a star, a snowflake. Oh, I see". Elena then created a chain structure with the magnetic models and shook it. They saw that the chain structure was unstable compared to ring structures, so they deduced that snowflakes would not contain chain structure. When observing the cyclic structure, Elena pointed at an O atom and discussed the four hydrogen bonding around oxygen.

Elena: "[Pointing at an O atom] Like, um, it's got the four, it's got four hydrogen bonds."

Fiona: *"[…] Yeah, I know what you're saying. Which one? This one? Yeah, so that would have two hydrogen bonds, but it's bonded to four hydrogens."*

Elena still seemed to harbour her alternative understanding of hydrogen bonding. Now, not just by pointing, Fiona also manipulated the models to show Elena how it was easier to separate O-H between water molecules than O-H within water molecules. After being prompted, Fiona and Elena tried to add as many water molecules as possible and created a tetrahedral. However, Fiona and Elena did not further discuss why there were four binding spots and did not seem to relate the 3D tetrahedral with their earlier exploration of the cyclic structure.

Using two and then multiple magnetic models, Fiona and Elena applied their individual prior understanding to support each other. With Fiona's support when exploring the magnetic models, Elena could show the difference between hydrogen and covalent bonds in her post-diagrams. For Fiona, explaining the basic concepts to Elena seemed to help her carefully consider what she observed with magnetic models. This can be seen in Fiona's representation of the distance between water molecules in her post-diagrams (Table 4.2), even though she saw the models directly touching each other. Fiona and Elena's interaction with magnetic models showed that pairs with mixed prior knowledge could use the magnetic models to interrogate and support each other's conceptual development.

4.3.3 Conceptual Understanding After Activities With Magnetic Models

For the concept of hydrogen bonding, both changed their understanding of hydrogen bonding. Fiona changed from drawing two to four water molecules, forming hydrogen bonding with a central molecule. She maintained to show that there were certain distances and angles between water molecules, and she added that some of the molecules were "coming out and into the page". Elena's explanation of the interaction between water molecules changed from O-O to O-H interactions. Using different colours, she showed the difference between "bonds within molecules" (blue lines) and "bonds between molecules" (black lines). After drawing multiple water molecules, she realised that some of them were close enough to form hydrogen bonding and connected them with a red line that she labelled "close proximity interaction". Unlike Fiona, Elena was drawing a flat structure, not 3D.

For the concept of snowflake formation, Fiona and Elena highlighted that the branches of snowflakes originated from tetrahedral structures instead of a chain structure like they originally thought. Elena mentioned cyclic structures in her explanation of snowflakes but did not elaborate on how they connected with tetrahedral. Her gesture and explanation suggested that the expansion of molecular structure happened on a 2D plane.

> Elena: *"It gives you a better idea of how they, like, sprawled from the middle [pointed at her drawings of water molecules and spread her fingers]."*

4.3.4 Conceptual Understanding Before iVR Activities

For the concept of hydrogen bonding, Fiona and Elena explained that there should be an optimal distance and angle between two water molecules to form hydrogen bonding. Elena added annotation to show the optimum angle between "O-H-O-H" chains and the distance between water molecules. Fiona reiterated that her drawing is 3D, with some molecules going in and out of the page, and she did not change her drawing.

For the concept of snowflake formation, Fiona and Elena's explanation did not change from before. They still focused on the branching of snowflakes on a flat plane.

4.3.5 Interaction in iVR

Fiona had a better idea of the 3D spatial arrangement of water molecules than Elena before the iVR activity. Inside the iVR space, Fiona and Elena enthusiastically explore the simple structures to discuss salient features, such as the shape of the 3D structures in relation to snowflakes. However, they struggled to handle different concepts when manipulating complex structures. As a result, Fiona and Elena quickly moved to the next tasks without providing scientific reasoning beyond the observable features of the complex structure.

Fiona and Elena seemed to have a good time forming hydrogen bonding with two water to discuss the 3D orientation of water molecules. They laughed a lot during their exploration and looked around the space and at each other's avatars. This pair overlapped O and H atoms as if trying to reenact their actions with magnetic models. Fiona, who showed better appreciation of the distance and position of lone pairs, could finally form hydrogen bonding after several trials. When Elena could not form the hydrogen bonding, Fiona supported Elena as she did during the activity with magnetic models. In iVR, they took turns to rotate the molecules extensively and walked around to align O and H atoms at a certain distance. Because Fiona and Elena focused on establishing the "rule" of hydrogen bond formation (O-H attraction), they did not engage in discussion beyond the salient colour and thickness of hydrogen bonding. When prompted about bond strength, Fiona and Elena aimed to create a thick green bond without explicitly discussing the implication of angle and distance towards the strength of hydrogen bonding.

During the tetrahedral task, Fiona and Elena continued to show enjoyment and used multiple 3D water molecules to predict and experiment with the maximum number of water molecules. Even though Fiona and Elena already explored tetrahedral structure during the activity with magnetic models, they still predicted two instead of four hydrogen bonding per water molecule. This is perhaps because their exploration of tetrahedral was not initiated by themselves, and they did not spend time discussing it with each other during the activity with magnetic models. In iVR, both grabbed, rotated, and observed a molecule to correct themselves and explain it was four hydrogen bonding instead of two. As shown in the following exchange:

Elena: *"So you see how like it is that bit. And that bit? [pointing at two H atoms] That's where the hydrogen bonds are like go, right?"*

Fiona: *"Huh. Now, like, it can connect up with those [pointing at lone pairs]. It's like this."*

Elena: *"No… [rotating the molecules] Oh, yeah! Four!"*

By sharing and manipulating the water molecules together, Fiona and Elena challenged each other's hypothesis and developed a better understanding of the 3D spatial arrangement of water molecules.

Fiona and Elena expressed confusion when constructing and observing complex structures. Both struggled when constructing the single layer of ice. So, they decided to move on to the next task after only connecting two clusters and excitedly mentioned the chair conformation (or "zigzag" in their terms) and hexagonal structure. In the ice lattice vs. snowflakes task, they flipped, rotated, and superimposed a snowflake to the whole ice lattice, attempting to find a matching shape. Fiona tried looking at a portion of the lattice (the edges) to explain the branches, but Elena seemed unconvinced and pressed the submit button. When given information about the size of snowflakes, both explained that because the lattice only represents a small part of a snowflake, it was impossible to use it to explain the shape of snowflakes.

Elena: *"[Reading instructions] Compared with numbers and discuss its implications. Well, because it's really big, how do you know which way it goes [pointing at lattice]?"*

Fiona and Elena explained that water molecules arranged themselves in a 3D hexagonal formation, which resulted in a six-fold symmetry of snowflakes in the post-interview. Their drawing resembled the connected two clusters of water molecules they made in iVR. Because they focused on the observable match between molecular and macroscopic structures, these students seemed to benefit more from the simple structure tasks. Without a relevant understanding of molecular scale difference and growth, this pair's strategy to simply match the molecular shape with the shape of snowflakes did not seem to work as the molecular structures became complex.

4.3.6 Conceptual Understanding After iVR Activities

For the concept of hydrogen bonding, Fiona and Elena did a collaborative drawing showing hydrogen bonding (red) as interactions between O-H interactions of different water molecules. A different colour (black) represented the bond within water molecules. Both explained that their drawing is 3D, but it was hard to tell which parts were exactly going into and out of the page, as Fiona explained:

Fiona: *"Like, that looks like it's going down. But it's probably, like, coming out towards you or something. So, it's like hard to decide where are you meant to put them on the page?"*

They were trying to draw hexagons but ended up with a squarish structure. Unsatisfied, Elena then tried to draw her own hexagonal structure. She ended her attempt halfway and admitted that it was difficult to decide the direction of the "branching" on non-3D media, such as paper.

For the concept of snowflake formation, Fiona and Elena both explained the hexagonal symmetry of snowflakes in relation to the hexagonal structure formed by water molecules through hydrogen bonding. Fiona included ideas about tetrahedral and layers to show her understanding of the 3D aspect. However, Elena explained the hexagonal structures expanded horizontally to eventually form branches of snowflakes. When Fiona mentioned "layers of hexagons", Elena looked confused and asked Fiona about it. Elena's confusion indicates only Fiona developed an appreciation of 3D lattices in relation to snowflakes.

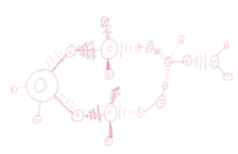
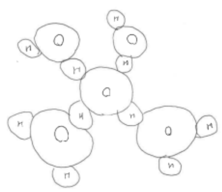
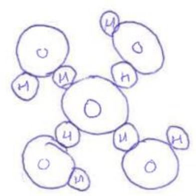
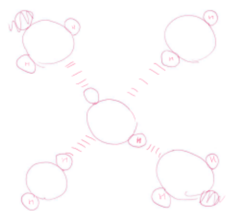
4.4 Nigel and Jasper

4.4.1 Conceptual Understanding Before Activities With Magnetic Models

For the concept of hydrogen bonding, Nigel and Jasper used the term "hydrogen bonding" to describe the interaction between water molecules and represented hydrogen bonding as dash lines. They explained hydrogen bonding is formed because slightly negatively charged O atoms (δ^-) attract slightly positively charged H atoms (δ^+) of different water molecules. Initially, both did not consider the lone pairs and thought the whole O atoms were partially negatively charged. When prompted further, Nigel decided that each free electron on the O atoms could attract another water molecule. Jasper's drawing was slightly different because he initially considered both H atoms as one whole positive area and the whole O atom as one negative area. However, he changed after hearing Nigel's explanation to consider individual H atoms and individual free electrons of O atoms. While Nigel consistently used "attraction between water molecules", Jasper also mentioned "gaining or sharing electrons" when explaining the interaction between lone pairs and H atoms of different water molecules.

Table 4.3

Change in Nigel and Jasper's Diagrams of Hydrogen Bonding

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Nigel	 Category B	 Category C	 Category C	 Category D
Jasper	 Category B	 Category A	 Category A	 Category D

For the concept of snowflake formation, Nigel and Jasper noticed the six-branches and the symmetry of the snowflakes. Both gave a general explanation of how, due to different environmental conditions, water molecules would bond differently to each other to form various structures (patterns) of snowflakes.

4.4.2 Interactions With Magnetic Models

Instead of four, Nigel and Jasper drew six water molecules around a central water molecule, trying to mimic the six branches of snowflakes. Using the magnetic models to test their hypothesis, this pair experimented with adding as many water molecules as possible to one water molecule and discovered the tetrahedral formation to explain the branching of snowflakes. However, Nigel and Jasper exhibited divergent understanding of the nature of hydrogen bonding because they did not talk about it extensively with each other during this activity.

Equipped with knowledge about O-H attraction, Nigel and Jasper used magnetic models to explore the directionality of hydrogen bonding. At first, this pair (mostly Nigel) briefly showed and explained that O-H attracts and the O-O and H-H repulse to confirm their understanding. Then, they rotated the models and discussed the position of lone pairs and H atoms. After being prompted, this pair pushed two models of water molecules across the table. By observing how the magnetic models behave when pushed across the table, this pair discussed that water molecules would orient themselves so that the O and H atoms were aligned to accommodate the formation of hydrogen bonding.

With more models of water molecules, Nigel and Jasper have more opportunities to test their hypothesis about molecular formation. As if they were trying to replicate their pre-interview diagrams, Nigel and Jasper tried to attach more than four water molecules to the central one only to find out they could not, as shown in the following exchanges:

Jasper: "*I got four all bonded, and I'm trying to get to that central one, and that's not …"*

Nigel: "*I guess it's impossible to have six [water molecules] to one."*

Nigel and Jasper rotated the models, discussed the 3D direction of each of the four hydrogen bonding around the central molecules, and recognised that it was a tetrahedral formation, as explained by Nigel:

Nigel: *"So, it's like almost like it's not a flat plane. It's got sort of bents and stuff in between. Yeah. And we can see that, like, not all the hydrogens or not all the molecules are in the same sort of orientation."*

The discussion about how water molecules orient themselves continued when they explored a cyclic structure. When the interviewer asked about the stability of cyclic structures, only Nigel responded. He explained that pentagons and hexagons were relatively stable compared to other cyclic structures. Jasper then mentioned orientation. So then, this pair began discussing how water molecules orient themselves to form hydrogen bonding in various shapes, such as cyclic shapes. They seemed not to find the cyclic structure relevant to tetrahedral and snowflake structures.

Nigel and Jasper's interactions with magnetic models showed that they were driven by their partial understanding of the role of lone pairs. Their exploration helped them to establish the idea of tetrahedral structures. However, Jasper did not represent hydrogen bonding as dash lines, and his explanation suggested a mix-up between hydrogen and covalent bonds. This is perhaps because Jasper saw magnetic models touching each other without any gaps and accepted them as true representations of water molecules. On the other hand, Nigel explicitly distinguished inter and intramolecular bonds. This divergent understanding may be because Nigel mostly did the talking during this activity. Jasper said in the post-interview, "I mean, instantly, my anxious mind goes panic. I'm in a test." Jasper perceived the activity with magnetic models as an individual test instead of a collaborative work, which caused him to panic and not contribute much to the discussion. Without talking to each other, it may be difficult for these students to monitor each other's learning and create a joint understanding.

4.4.3 Conceptual Understanding After Activities With Magnetic Models

For the concept of hydrogen bonding, both changed their drawing to show a central water molecule interacting with four instead of six water molecules. However, Nigel referred to his drawing as square (not 3D). Nigel continued to show the polarity of the molecules in his drawing, but Jasper did not. Jasper explained that the water molecules share electrons, not lose or gain electrons. This explanation suggests that Jasper might have an unclear understanding of the difference between hydrogen bonding and covalent bonds. Unlike Nigel, Jasper did not represent hydrogen bonding as lines.

For the concept of snowflake formation, Jasper explained the shape of snowflakes as a result of water molecules interacting with each other to make a structure. His explanation was broad, like before the activity with magnetic models. On the other hand, Nigel reasoned that the four "branches" of water molecules stemming from a central molecule would expand to eventually form hexagonal snowflakes.

Nigel: *"Since we're branching out, [so] you go from one to four to 16. To think this sort of structure eventually going from a square to a hexagon."*

Nigel changed his earlier explanation to include more specific ideas, but the idea of 3D expansion, including the relation between tetrahedral and hexagons, was still unclear.

4.4.4 Conceptual Understanding Before iVR Activities

For the concept of hydrogen bonding, Nigel still showed that one water molecule could interact with a maximum of four other water molecules. Nigel pointed out that there were optimal angles and distances between water molecules. Nigel might have an alternative preconception of the optimal angle as O-H instead of O-H-O (like Ana did). On the other hand, Jasper highlighted the attraction between O and H atoms. Some of the water molecules in his drawing were missing H atoms. He explained his drawing about O atoms capable of attracting four H atoms. Jasper's explanation suggests that he did not clearly distinguish between hydrogen bonding and covalent bonds.

For the concept of snowflake formation, Nigel and Jasper explained that the water molecules would interact in specific orientations, which resulted in the "nice" symmetry of snowflakes. And the variation of patterns was the result of variation of orientation as the water molecules "froze into place".

4.4.5 Interaction in iVR

Nigel and Jasper highlighted four as the maximum number of hydrogen bonding per water molecule before their interaction in iVR. However, both were missing the 3D aspect, and Jasper even mixed hydrogen bonding with covalent bonding. In iVR, Jasper changed from being reserved to more confident in sharing his ideas. Together, these students established the nature of hydrogen bonding in the context of a 3D lattice of ice and the six-fold symmetry of snowflakes in iVR.

Nigel and Jasper exhibited their pre-existing social dynamic and two-dimensional preconceptions when forming hydrogen bonding in iVR. Nigel, who was more confident in using chemistry terminology, dominated the discussion and took control of the water molecules. Although Jasper voiced his opinion more in iVR, it did not seem enough to overcome Nigel's dominance. For example, Jasper was aiming for 0° off-axis for a strong hydrogen bond, but Nigel only acknowledged Jasper's idea once before going back to his preconception of 180° as the optimum angle, as shown below:

Jasper: *"I'm trying to get this on zero [adjusting the molecules]."*

Nigel: *"I think I hit zero just like before. […] So [the angle] matters as long as it's 180, I think it's fine. […] Perfect. Yeah, I think 180, do you think it's 180?"*

In strengthening the bond, Nigel took control and focused on one aspect, the angle, by aligning lone pairs and hydrogen atoms and looking at the off-axis value. Interestingly, the impact of the distance on bond strength was less discussed, even though Jasper hinted about it.

As more water molecules became available for exploration, Nigel and Jasper's interactions became more collaborative and explorative. After quickly completing the tetrahedral task to confirm their understanding, this pair began extensively exploring the iVR space by grabbing and rotating them, walking around, and even bending their bodies. Jasper also shared his ideas more in the task with complex structures. They do not want to give up when they face a challenging task. Perhaps they treated the task as a puzzle game, as Jasper said when doing the single-layer task:

Jasper: "*No, no, I think it's (clusters) meant to be different. We need to resolve it. I played enough video games*."

Determined to solve the puzzle, they assumed different positions, walked and bent down to find new information. Due to their extensive exploration of the complex structures, this pair discovered various ideas of the 3D spatial arrangement of water molecules, such as hexagonal patterns and the alternating arrangement of lone pairs and H atoms. Their appreciation of 3D spatial arrangement can be seen in Nigel's drawing of 3D hexagons and Jasper's drawing of tetrahedral after iVR. Seeing the hydrogen bond explicitly as a colourful stick might benefit Jasper. He improved his previous drawing to include the difference between inter and intramolecular bonds.

In terms of snowflakes, these students began relating the molecular structure and snowflakes when prompted to do so in the ice lattice vs. snowflakes task. When they placed the snowflakes onto the ice lattice, they found that the snowflakes' symmetry matched the lattice's hexagonal pattern. Nigel and Jasper further explored the edges of the lattice and found that the protruding parts could be the stem of the snowflakes' branches. Jasper initially thought that the snowflakes were smaller than the lattice. But then, with the info from the instruction screen, Nigel and Jasper discussed that the ice lattice was a minute part of snowflakes.

Based on Nigel and Jasper's interaction in iVR, it seemed that exposing students, especially the confident ones like Nigel, to new, unfamiliar setups/ structures in iVR could help them change their 2D preconceptions into an understanding of 3D molecular interactions. The unfamiliar, complex structures/tasks and the absence of an interviewer ("powerful" figure) could also benefit quiet students like Jasper in voicing their ideas to their peers. With a specific prompt at the end of the iVR activity, these students could use the ice lattice structure to better understand the 3D hexagonal structure to explain the formation of snowflakes.

4.4.6 Conceptual Understanding After iVR Activities

For the concept of hydrogen bonding, Nigel and Jasper represented hydrogen bonding as dash lines between O and H atoms of water molecules. Both now have considered the tetrahedral geometry of water molecules. Jasper showed it by drawing H atoms and the hydrogen bonding of the central water molecule perpendicular to each other. In addition to showing hydrogen bonding (as dash lines) differently from covalent bonds, Jasper's drawing implied that hydrogen bonding is longer than covalent bonds. In addition to the 3D aspect, Nigel explained that water molecules interacted in 3D orientation to form a stable hexagonal shape, as he explained:

> Nigel: "*Once again, like it's a proper hexagonal shape. Now, we can see the various like sorts of like planes of things. So, we can see like these hydrogens are tilting out of the page.*"

For the concept of snowflake formation, Nigel and Jasper explained the six-fold symmetry of snowflakes due to the 3D hexagonal pattern found in the lattice. Nigel gave an extended explanation by including the step-by-step journey of polar water molecules hydrogen bonded to each other to eventually form a 3D lattice. Both also included information about environmental conditions to explain the variation of snowflakes' patterns.

4.5 Tiana and Renee

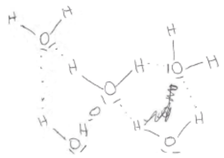
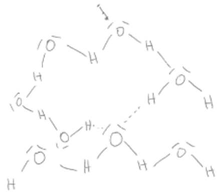
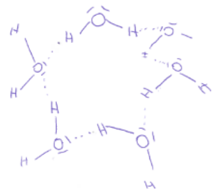
4.5.1 Conceptual Understanding Before Activities With Magnetic Models

For the concept of hydrogen bonding, Tiana and Renee described the interaction between water molecules as hydrogen bonding – an attraction between the partially negatively charged lone pairs on O atoms and the partially positively charged H atoms of different water molecules. However, Tiana wrote δ^+ for both O and H atoms. Both drew four water molecules as the maximum amount of interaction, but they did not mention any three-dimensionality of their drawings. Both represented hydrogen bonding as dash lines, and it was drawn at an angle, at various lengths – shorter, similar, or longer than a covalent bond.

For the concept of snowflake formation, both Tiana and Renee drew attention to the six-branches of snowflakes. Tiana reasoned that the six branches of snowflakes originated from six V-shaped water molecules bonded in particular angles. Renee agreed and reiterated Tiana's explanation.

Table 4.4

Change in Tiana and Renee's Diagrams of Hydrogen Bonding

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Tiana	 Category C	 Category C	 Category C	[Collaborative drawing with Renee] Category A
Renee	 Category C	 Category A	 Category C	 Category A

4.5.2 *Interactions With Magnetic Models*

Tiana and Renee showed a clear understanding of hydrogen bonding by drawing a *flat* structure of four water molecules around a central molecule before the activity with magnetic models. However, their exploration of magnetic models made them question the existence of 3D tetrahedral structures in nature. Instead, they only found similarities between the *flat* hexagonal structures and the *flat* hexagonal snowflakes.

With two models of water molecules, Tiana and Renee made a joint effort to find similarities between the molecular structures and the six branches of snowflakes. The exhibited teamwork was perhaps because Tiana and Renee knew each other from their laboratory session and acknowledged that they both had a reasonable understanding of hydrogen bonding. After explaining the reason for the attraction and repulsion between two water molecules, this pair shared their water molecules to explore the possibility of six water molecules interacting with a water molecule. These students had previously explained that snowflakes have six branches. Therefore, they tried to find the reason using magnetic models. As commented by Tiana while she observed the models to find possible areas for attraction:

Tiana: *"Like, I'm starting to assume with the snowflake thing, that's [pointing at models] going to be 6. So maybe you can … [rotate the models to find six binding spots]."*

Not satisfied with only having limited magnetic models among them, this pair were eager to have more water molecules to play with.

Tiana and Renee found a structural match between hexagonal structures and snowflakes but could not figure out how tetrahedral structures fit into their ideas of the six-fold symmetry of snowflakes. With more models of water molecules, this pair immediately attached as many water molecules as possible to the centre water molecule. They found that attaching more than four water molecules to the centre water molecule was impossible. Not seeing the connection between tetrahedral and snowflakes, Renee then gave an idea to make a flat structure because snowflakes are flat:

Renee: "*But snowflakes are flat, aren't they? So, maybe let's combine those ones. So, we make it as flat as we can go. [Make hexagonal structures with Tiana] Oh, there we go. Now we have snowflakes! We have a ring around there."*

When prompted to think about the tetrahedral structure they discovered earlier, they highlighted that snowflakes are flat, so the molecular structure should be flat. They attempted to create a lattice stemming from a tetrahedral. However, because they could not find a similarity between the lattice and snowflakes, Tiana and Renee concluded that a flat hexagonal structure is most likely to be found in a snowflake.

Tiana and Renee were driven by the idea of hexagonal symmetry to manipulate magnetic models. By finding structural matches at molecular and macroscopic levels, Tiana and Renee changed from highlighting the tetrahedral structure to highlighting the hexagonal structure to explain the shape of snowflakes. Similar to previously described pairs, this pair seemed to accept that magnetic models would behave exactly like water molecules. This behaviour suggests that students might need to mindfully observe and remind themselves of what was and was not represented by the magnetic models.

4.5.3 Conceptual Understanding After Activities With Magnetic Models

For the concept of hydrogen bonding, both wanted to show that water molecules could form a hexagonal structure and explained it as more stable than tetrahedral. Tiana still represented hydrogen bonding as dash lines between O-H atoms of different water molecules. However, for the last hydrogen bonding, she quickly connected O with O atoms of different water molecules to complete her cyclic structure. In contrast, Renee's drawing comprised O-H connections without differentiation between hydrogen and covalent bonds.

For the concept of snowflake formation, despite knowing about the 3D tetrahedral structures, both were adamant that it was unlikely to be found in snowflakes. Looking at their models of hexagonal structure, both explained that the hexagonal snowflakes originated from the horizontal expansion of hexagonal structures.

Tiana: *"Yeah, why is it six [point at the hexagonal structure]? So, it's more stable when they're just, like, longer [spreading]. Yeah. And flatter than like bulky."*

4.5.4 Conceptual Understanding Before iVR Activities

For the concept of hydrogen bonding, both still explained that water molecules interacted to a stable hexagonal structure. They also highlighted that the optimum O-H-O angle is 180°. The length of hydrogen bonding was drawn similarly to the covalent bond and was not verbally elaborated like the angle aspect. Renee realised the error in her previous drawing and explained the alternating arrangement of intermolecular forces (dash lines) and covalent bonds (solid lines) in a hexagonal structure.

For the concept of snowflake formation, neither student changed their explanation about the relation between the hexagonal structure and the hexagonal shape of snowflakes.

4.5.5 Interaction in iVR

Before the iVR activity, Tiana and Renee maintained their explanations of hexagonal-hexagonal parallel between *flat* molecular and *flat* macroscopic structures. With iVR, these students explored 3D complex structures to change their prior two-dimensional ideas of molecular structures and include 3D aspects in their explanation of hydrogen bonding and snowflakes.

Tiana and Renee's prior understanding of hydrogen bonding helped them swiftly complete the tasks with simple structures. When connecting two water molecules, they recognised the meaning of the text (distance) and the visual cue to explain the implication of angle and distance for a strong hydrogen bond. However, this pair kept mentioning 180° as the optimal angle. As noted by Tiana:

Tiana: "*So, that's the distance, and that's off-axis by that much; it needs to be 180.*"

This pair correctly predicted four as the maximum number of hydrogen bonding per water molecule during the tetrahedral structure task. However, these students were again adamant that a tetrahedral structure was unlikely to be present in a lattice (snowflakes). As explained by Renee:

Renee: *"The maximum number of hydrogen bonds. So, they can form four. But they're more stable at three."*

Like Nigel (section 4.4.5), students who seemed confident with their clear prior knowledge tend to hold on to their preconceptions when encountering familiar structures in iVR.

Unlike the two water molecules and tetrahedral tasks, the following complex structure tasks were new and challenging for Tiana and Renee. In constructing the complex structures, they also had to consider other 3D aspects beyond the O-H connection between two water molecules. Their heavy reliance on preconceptions might explain why Tiana and Renee did not explore much and struggled to find new information to construct the single layer successfully. They also seemed to want to give up, as shown by Renee:

Renee: *"I don't think we did it right because this thing shouldn't be up there. I don't want to do it again."*

Instead of coming up with their own strategy, this pair relied more on hints from the researchers after receiving the first hint to complete the task. After successfully completing the single layer, they directly proceeded to the next task without much discussion of the structures.

Seemingly learning from their experience in the single-layer task, Tiana and Renee extensively rotated the structure and changed their position to construct an ice lattice successfully. Renee even seemed more immersed in the task, so she hit a physical wall when she walked around. Assuming different positions, Tiana and Renee exchange information about what they observed from their angle. As shown in their conversation when constructing the lattice:

Tiana: *"If we look at the way the molecule is at the bottom, this doesn't match."*

Renee: *"[Standing at opposite side of the room] Well, it does. Doesn't it?"*

Tiana: *"No, because if you look, there's a dot and then …"*

Renee: *"Ooh, it's like straight on. So just shuffle it this way [gesture the direction]. That one that's too far."*

Unlike during the single-layer task, this pair spent time observing the structure when they successfully constructed the ice lattice without external hints. Perhaps this self-driven experience of building the 3D ice lattice was most memorable for them, so they tried to put it in their drawing after iVR.

Using the 3D lattice, Tiana and Renee appeared to finally change their preconception of flat hexagons. They noticed the hexagons on the lattice were on a different plane (3D) and could be seen from every angle. After overlaying snowflake structures on the hexagonal pattern of the ice lattice, this pair confirmed their hypothesis about the six-fold symmetry of snowflakes. In addition to the findings about hexagons, Tiana and Renee were also able to discuss the scale and the probability effect in relation to the growth of snowflakes.

As seen above, Tiana and Renee's interactions with simpler structures were a mirror of their previous interactions with magnetic models. When Tiana and Renee interacted with complex ice lattices in iVR, they finally realised the vertical and horizontal expansion of 3D hexagonal structures in connection to the six-fold symmetry of snowflakes. However, their post-diagrams (Table 4.4) showed an unclear representation of water molecules and hydrogen bonding. Perhaps the complexity of the ice lattice was overwhelming for these students, so they were having difficulty representing the hydrogen bonding between water molecules in the context of an ice lattice on paper.

4.5.6 Conceptual Understanding After iVR Activities

For the concept of hydrogen bonding, Tiana and Renee explained that interactions between water molecules resulted in both tetrahedral and hexagonal formation. However, they expressed confusion about representing their ideas on paper. Both drew O-H connections but not between water molecules. They explained that one water molecule could attract four other water molecules (three in a horizontal direction and one molecule in a vertical direction) but were unable to illustrate it in relation to hexagonal formation, as Tiana elaborated:

> Tiana: *"That's the base layer [pointing at their drawing in red]. And then that's the fourth one [pointing at the black O atoms in the middle] because, like, three bonds sit on one level, and then the fourth one is coming up."*

For the concept of snowflake formation, Tiana and Renee realised that they were stuck on thinking that hexagonal structures would expand horizontally before iVR. After iVR, they explained how water molecules would hydrogen bond to form hexagonal structures that also expand vertically to eventually form snowflakes with six-fold symmetry. Like most pairs, they also mentioned the environmental factor.

> Renee: "*Due to the positioning of the hydrogen bonds and the shape of the lattice that forms when water freezes, which forms hexagonal rings. And then those build upon each other. And then depending on the other factors, like temperature, variations in the environment will affect whether it's like a fast-growing one or smaller."*

4.6 Kenan and Pascal

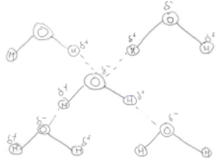
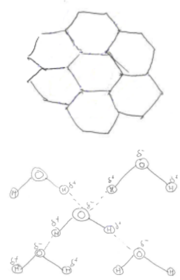
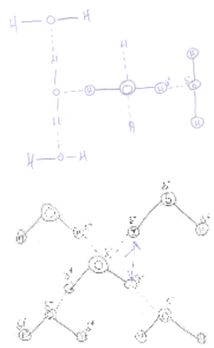
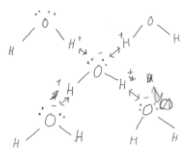
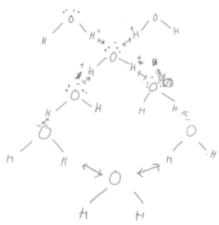
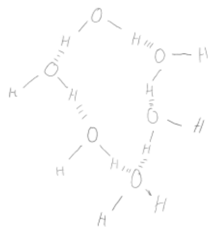
4.6.1 Conceptual Understanding Before Activities With Magnetic Models

For the concept of hydrogen bonding, Kenan and Pascal started the activity with a clear understanding of hydrogen bonding, like Tiana and Renee. Both assigned positive charges for H atoms and negative charges for O atoms. Both explained that the maximum number of water molecules interacting with one central water molecule is four (two to each of H atoms and two to each of lone pairs of O atoms). Kenan mentioned tetrahedral but was unsure what it meant in relation to the bent shape of water molecules. Pascal explained that tetrahedral refers to the position of two lone pairs and the two H atoms around an O atom of a water molecule. However, he did not elaborate on the 3D aspect of his final drawing.

For the concept of snowflake formation, Kenan and Pascal noticed that each snowflake was unique but had "repeating patterns". They seemed unsure exactly how the snowflake got its shape, so they gave a vague explanation that the water molecules would freeze in specific crystalline structures.

Table 4.5

Change in Kenan and Pascal's Diagrams of Hydrogen Bonding

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Kenan	 Category C	 Category C	 Category A	 Category D
Pascal	 Category C	 Category D	[Made no changes from the previous diagram] Category D	 Category D

4.6.2 Interactions With Magnetic Models

Kenan and Pascal started the learning activity with a clear understanding of hydrogen bonding on a 2D plane. This pair discovered hexagonal structures and attempted to create a 3D lattice comprising a hexagonal subunit using the magnetic models. However, the lattice structure crumbled, and they resorted to a more stable *flat* network of hexagonal subunits to explain the hexagonal shape of snowflakes.

Using two models of water molecules, Kenan and Pascal explored the orientation of four binding spots on a water molecule. Similar to pairs that had a clear understanding before the activity with magnetic models, Kenan and Pascal went beyond explaining the O-H attraction and O-O and H-H repulsion between water molecules. They also rotated the models to confirm that they were right about four as the maximum number of hydrogen bonding. But they also noticed that, unlike their 2D pre-diagrams, the models showed the 3D orientation of the four hydrogen bonding, as discussed by Kenan and Pascal:

Pascal: *"And I think we were right because there's two negatives."*

Kenan: *"Yeah. So, these would be the two lone pairs. […] Yeah, it's also kind of like, it doesn't look exactly like how we drew it. Kind of has to be… I don't know how to explain it. It [the molecules] has to be perpendicular to how we drew it."*

They then wished they had more water molecules to see the complete four hydrogen bonding around a central water molecule.

Using more water molecules, Kenan and Pascal shared the models with their partners to explore more complex structures, including stacked rings/lattices. They started discussing the tetrahedral subunit in relation to snowflakes, as Kenan said, "and this [tetrahedral] unit would be repeated infinitely". Both then combined their tetrahedral structure and noticed six-membered ring structures. Seemed surprised and curious about the hexagons, they stripped down the lattice to create individual hexagonal subunits and discovered the link with snowflakes, as shown here:

Kenan: "*You kind of get rings of six. Hmm. Interesting! [Why?] Because there's six in there [pointing at the picture of the snowflake]."*

Following their earlier exploration of 3D lattice, they now tried to create a lattice by combining six-membered rings, but the lattice crumbled. Because both knew ice should be stable, they made a network of rings on a 2D plane that looked more stable than the crumbling 3D lattice. As shown in their discussion:

Kenan: *"So, I guess if we just go back to this [a hexagon] and just kind of try to build it [on a 2D plane]. Because that [3D lattice] wasn't stable like that, we had a lot of sketchy connections."*

Pascal: "*We have kind of six [membered] rings. Maybe we can add that somewhere."*

Kenan: *"Well, that [network of hexagons] kind of worked. And we've got repeating units with six. I think that's stable. Everything looks right."*

With this observation, Kenan and Pascal explained that the hexagonal symmetry of snowflakes originated from the horizontal expansion of a network of molecular hexagonal structures.

Kenan and Pascal better understood the growth of 3D structures to explain macroscopic structures, unlike previous pairs who focused on a direct match between molecular and macroscopic structures. However, the magnetic models were limited in supporting Kenan and Pascal's exploration of the 3D expansion of tetrahedral and hexagonal subunits. Without step-by-step guidance, it was difficult to create a stable lattice. Like other pairs who trusted the models as true representations of water molecules, they then accepted the more stable flat network to explain the horizontal expansion of snowflakes. Despite being strangers, they seemed comfortable sharing their ideas and their models. Sharing models allowed the construction of complex structures and discussion among the students without much prompting from the interviewer.

4.6.3 Conceptual Understanding After Activities With Magnetic Models

For the concept of hydrogen bonding, in terms of hydrogen bonding, Kenan was happy with his previous drawing. He explained that the molecules on his drawing should be rotated 90 degrees (out of the page), perpendicular to the central water molecule, resulting in a 3D structure. However, he proceeded to draw a network of flat hexagons, which indicates he was unsure about the 3D spatial arrangement of water molecules on a bigger scale. In contrast, Pascal added three more water molecules to create a hexagon. He explained that the water molecules at the bottom of his original drawing should be tilted out to accommodate the formation of a hexagonal shape. He maintained to represent hydrogen bonding as the attraction between O and H atoms of different water molecules, but sometimes the water molecules were drawn very close to each other.

For the concept of snowflake formation, Kenan and Pascal discovered that water molecules could form a hexagonal structure and used that discovery to explain the hexagonal shape of snowflakes. By spreading his arm across the table, Kenan explained how a network of hexagonal structures would expand horizontally in six directions, resulting in a six-fold symmetry of snowflakes.

4.6.4 Conceptual Understanding Before iVR Activities

For the concept of hydrogen bonding, Kenan explained that his previous drawing of a network of hexagons was incorrect because it was not 3D. In his attempt to draw 3D structures, he drew hydrogen bonding as O-O interactions instead of O-H interactions of different water molecules. Meanwhile, Pascal made no changes to his drawing and reiterated that his drawing is 3D.

For the concept of snowflake formation, Kenan and Pascal began to doubt their earlier explanation of hexagonal snowflakes. They realised that water molecules interact in 3D space as a tetrahedral and did not see their connection with the six-fold symmetry of snowflakes.

4.6.5 Interaction in iVR

Kenan and Pascal had a clear understanding of hydrogen bonding but were uncertain about the link between 3D molecular structures and snowflakes before their interaction in iVR. Following the task progression from simple to complex structures in iVR, this pair continuously manipulated the structures, walked around, and discussed the optimal 3D arrangement of water molecules. When constructing and observing the complex structures, this pair realised the connection between tetrahedral and hexagonal subunits in relation to snowflakes' formation.

Kenan and Pascal used visual and text cues to make sense of 3D spatial arrangement during the simple structure tasks. This pair was one of the few pairs that could distinguish and link the meaning of visual cues (colour and thickness) with the text information (angstroms and off-axis). This was achieved by systematically adjusting the angle and distance between two water molecules. Making sense of the visual and text cues helped this pair to discuss the implication of optimal orientation when creating a strong hydrogen bond in iVR. During the construction of the tetrahedral, this pair continued to consider optimal 3D orientation. As Pascal said:

> Pascal: "*And they [point at hydrogen bonds] need to be evenly spaced. And that's why it is tetrahedral.*"

Rather than directly applying their previous learning, this pair adjusted their approach to adapt to the 3D learning environment. Perhaps because both had extensive iVR gaming experience, they appreciated the importance of walking around and talking to each other to gain different perspectives and new information.

Kenan and Pascal's extensive exploration helped them to notice various 3D molecules and construct complex structures successfully. With comments like "Wow!" and "That's pretty sick!"

Kenan and Pascal seemed excited to explore the complex structure, something they attempted to do with magnetic models but were unsuccessful. When constructing complex structures, they rotated the structures and discovered various 3D spatial arrangements, such as staggered hexagons and uniform lone pairs/hydrogens on each side. Kenan and Pascal also assumed different positions and reported what they observed to each other. This pair was one of the fastest pairs to successfully complete the construction of complex structures. Their extensive exploration helped them discover new ideas about 3D spatial arrangements, even those not found by other pairs. For example, Kenan recognised two types of water clusters during the single-layer task. Kenan and Pascal could single out a water molecule in the lattice to discuss the tetrahedral subunit by walking in and out of the complex structures.

Kenan and Pascal began discussing the link between molecular structure and snowflakes while exploring complex structures. Although both discussed hexagonal similarities at molecular and macroscopic (snowflakes) levels during the activity with magnetic models, they (especially Kenan) were unsure about the idea of a hexagon after realising that it was not 3D. In iVR, Kenan and Pascal reaffirmed their ideas of hexagon-hexagon parallel between molecular structure and snowflakes after consistently observing it in every complex structure task.

Pascal: "*It's six rings again.*"

Kenan: "*Ah, nice! Maybe you are right. Okay, so it is a hexagon. Let's check this out, alright. So, on alternating ones... [pointing at the staggered hexagonal structure].*"

With the snowflakes in their hands, Kenan and Pascal compared and concluded that all snowflakes were hexagons as a result of the hexagonal pattern of the ice lattice. They recognised that the lattice had a repeating pattern, including tetrahedral subunits, and could grow as more water molecules joined. However, they still wondered how the uniform repeating units resulted in the various patterns of snowflakes' branches.

As illustrated earlier, Kenan and Pascal's extensive exploration of the structures and consideration of each other's perspective helped them to find the optimal 3D arrangement of water molecules to explain the six-fold symmetry of snowflakes. In the post-interview, Kenan could finally explain the link between 3D tetrahedral and hexagonal structures after manipulating the ice lattice in iVR. On the other hand, Pascal did not explicitly discuss tetrahedral subunits after iVR. Maybe because Pascal was mostly building on Kenan's lead when constructing, observing, and discussing the complex structures in iVR, he did not find the need to repeat all of Kenan's explanations in the post-interview.

4.6.6 Conceptual Understanding After iVR Activities

For the concept of hydrogen bonding, Kenan and Pascal represented hydrogen bonding as dash lines between O and H atoms of water molecules. Both explained that the angle and distance need to be optimised to result in a 3D structure. In addition to his original drawing, Kenan provided another drawing to show the interaction of water molecules from a different angle (top view). He explained that the bent-shaped water molecules looked linear in his drawing because they were viewed from the top. Pascal showcased interactions of water molecules to result in a hexagonal formation. He realised that his drawing looked flat, so he explained with hand gestures that some of the water molecules were tilted in and out of the page.

For the concept of snowflake formation, Kenan recognised that tetrahedral subunits would expand, resulting in a 3D ice lattice with hexagonal patterns. He continued explaining that the lattice would get bigger as more water molecules joined, eventually resulting in the hexagonal shape of snowflakes. Pascal gave a shorter explanation focusing on layers of six-membered rings that continued to build on to form the six-fold symmetry of snowflakes. He did not imply tetrahedral subunits like Kenan.

4.7 Zeke and Turner

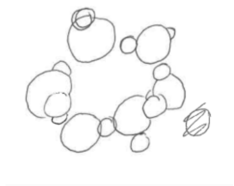
4.7.1 Conceptual Understanding Before Activities With Magnetic Models

For the concept of hydrogen bonding, Zeke and Turner explained that water molecules interacted through hydrogen bonding, which was an attraction between the lone pairs of O atoms and H atoms of different water molecules. To highlight his explanation of attraction, Zeke added δ^- to O atoms and δ^+ to H atoms. Zeke explained that water molecules would form hexagons in the lowest energy state, such as in low temperatures. Turner added that the distance between the water molecules would be minimal in freezing temperatures. Even though Zeke explained that his drawing of a hexagon was 3D, he was unsure how. When prompted to think about the maximum number of water molecules interacting with one, both explained it was four water molecules. Both drew wedges to show the 3D aspect of hydrogen bonding (Zeke) or water molecules (Turner). However, their drawing did not always align with their verbal explanation of a lone pair attracting hydrogen. Their explanation suggests that they were still unsure about the orientation of hydrogen bonding in 3D.

For the concept of snowflake formation, Zeke explained that snowflakes are hexagonal because water molecules would hydrogen bond with each other and organise themselves into hexagonal patterns. Turner, in contrast, simply agreed with Zeke.

Table 4.6

Change in Zeke and Turner's Diagrams of Hydrogen Bonding

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Zeke			[Made no changes from the previous diagram]	
	Category C	Category D	Category D	Cannot be categorised
Turner				
	Category C	Category C	Category C	Category D

4.7.2 Interactions With Magnetic Models

With a clear understanding of hydrogen bonding, Zeke (mostly) and Turner explained the shape of snowflakes in terms of water molecules packing close together to form a hexagonal structure. Due to Zeke's dominance during this activity, Turner's ideas, such as exploring 3D lattice, were not further elaborated. These students used the magnetic models to confirm Zeke's hypothesis that hexagonal structures were one of the most stable molecular structures and the reason why snowflakes have six-fold symmetry.

Zeke and Turner briefly interacted with two magnetic models to confirm their understanding of hydrogen bonding. After explaining the O-H attractions, they discussed that water molecules would orient themselves to form hydrogen bonding after pushing the models across the table.

They also pointed out the four binding spots (two lone pairs and two hydrogens) for forming hydrogen bonding. Zeke and Turner's interaction with two models of water molecules was typical for pairs with clear prior knowledge of hydrogen bonding. They seemed eager to play with more water molecules.

Zeke and Turner shared their magnetic models to test the stability of various molecular structures. These students were friends and had worked together before in class, which may be why they immediately shared the magnetic models that allowed them to construct more complex structures. They directly made ring structures and combined them to create a stacked ring structure with more models of water molecules. Interestingly, this pair did not attempt to create tetrahedral, perhaps because they were confident with their clear understanding of hydrogen bonding between water molecules. However, Zeke seemed more confident and led the exploration. Turner gave a short comment that the stacked ring structure is ice. Zeke wanted to see how water molecules would naturally interact, so he tore the lattice apart without building on Turner's comment. As shown in the following:

Turner: *"Yeah. We made ice."*

Zeke: *"I guess it's cool because it kind of shows, especially when you have like a lot of them together. [Begin to tear the structure apart] But what if we just take them more apart and just kind of just slap them all together?"*

They then threw a bunch of magnetic models on the table. The resulting structure was a chain structure, which they recognised as unstable. They then tested the stability of various ring structures by feeling the variation of magnetic strength when pulling the structures apart. As shown by Zeke's comment during the activity with magnetic models:

Zeke: *"Well, if you look at the five [membered ring], that's kind of like a small gap in between, like it's that kind of shows like it's a little bit is a bit less strong level. So, if I can make a six, six if I make a six and then try and pull the six [membered ring] apart, it takes quite a bit of force."*

The haptic feedback of magnetic models allowed this pair to deduce that pentagons and hexagons were more stable than other structures. Zeke and Turner could not decide which was more stable between hexagons and pentagons because the strength required to break them felt the same. In the end, they decided to use the hexagonal structure to explain the symmetry of snowflakes.

As seen above, Zeke and Turner seemed eager to share their models, which allowed them to explore more complex structures, like Tiana-Renee and Kenan-Pascal. However, because of Zeke's dominance and Turner's quiet nature, some of Turner's ideas, including a 3D lattice of ice, were not fully explored. In the post-interview, both copied the 3D cyclic model on paper, which caused them not to consider or represent the relative distance between water molecules. Similar to Tiana-Renee and Kenan-Pascal, this pair did not explain the vertical expansion of the structure, perhaps because of the same reason – not exploring the 3D lattice with a hexagonal pattern.

4.7.3 Conceptual Understanding After Activities With Magnetic Models

For the concept of hydrogen bonding, Zeke and Turner illustrated that water molecules formed 3D cyclic structures through hydrogen bonding. The hydrogen bonding was no longer represented as dash lines. Instead, both illustrated water molecules almost touched each other, like Ana. Some of the water molecules in Turner's drawing were missing H atoms, and thus, the hydrogen bonding was shown as interactions between O-O atoms of different water molecules.

For the concept of snowflake formation, both students highlighted that the hexagonal shape of snowflakes resulted from the growth of six-membered ring structures. They did not indicate any vertical expansion of the structure.

> Turner: "*I'll go with the understanding that the six [membered ring] structure is the strongest, and then you can even expand off the six. […] they are coming off and making larger branches.*"

4.7.4 Conceptual Understanding Before iVR Activities

For the concept of hydrogen bonding, Zeke did not make further changes to his diagrams except to reiterate that it is difficult to represent 3D structures on paper. Turner circled the top two water molecules to explain that water molecules interacted at optimal angles. However, he did not change the distance between the two water molecules.

For the concept of snowflake formation, Zeke and Turner did not change their explanation of snowflakes except by adding information about phase changes. Zeke elaborated that water molecules "fly everywhere" in the liquid phase and interact more with each other to form a "lattice" as the temperature gets lower.

4.7.5 Interaction in iVR

Before the iVR activity, Zeke and Turner explained hydrogen bonding in the context of cyclic structures, but the idea of expansion of the cyclic structure in the 3D direction was still lacking. Compared to the interaction of this pair before iVR, both contributed more equally to their exploration. By interacting in iVR, Zeke and Turner developed an understanding of the 3D spatial arrangement of water molecules to explain the shape of snowflakes.

Zeke and Turner's interaction during the simple structure task was similar to how they behaved in the activity before iVR. Zeke took control most of the time to test his ideas before giving the molecules to Turner. Like other pairs with extensive iVR gaming experience and good prior knowledge, this pair tried different configurations of water molecules to discuss the implications of angle and distance in forming strong hydrogen bonding. During the tetrahedral task, Zeke initiated the constructions of different cyclic structures (square, pentagons, and hexagons) to test their stability, as he did with magnetic models. Using the visual cue (colour and distance) to ascertain the strength of hydrogen bonding, they concluded that hexagons were the most stable out of the cyclic structures they tried to construct. As can be seen in Zeke's elaboration when this pair create pentagons:

Zeke: " *You can really see what this one does not want to do five [pointed at an orange hydrogen bond in pentagons]. I've got like one good bond, but then all the other ones that just like don't want to form [hydrogen bonds]."*

As observed in pairs with leader-follower dynamics, Zeke and Turner contribute more equally during the discussion and exploration of complex structures. Initially, Zeke took control of the construction of the single layer before involving Turner. Turner silently tried to construct the layers on his own. After a few minutes without progress, Zeke read the instructions again and asked Turner to join him in building the single layer. Unlike in the task with two water molecules and tetrahedral, these pairs seemed to realise that they could no longer simply rely on or confirm their prior knowledge. Both assumed different positions and successfully discovered the pattern to construct a single structure. They repeated their strategy for constructing the ice lattice. Both observed the structures to discuss the hexagons, zigzag structure, alternating lone pairs and hydrogen atom arrangement. After switching mode from passive-individualistic to more active-collaborative, this pair successfully constructed the complex structures. Both contributed to the discussion of 3D spatial arrangement of water molecules, as shown below:

Zeke*: "Just kind of like flat but also kind of, it's like a zigzag."*

Turner: *"Zigzag. You'll see another layer on top of here exactly the same [point at the uniform lone pairs and hydrogen on each side of the layer of ice]."*

Turner and Zeke's learning from these tasks can be seen in their drawing after iVR. Both were focused on the complexity of 3D lattices (zigzag and hexagons).

Zeke and Turner seemed to understand the extent of what can be explained from the ice lattice. When comparing the snowflakes and the ice lattice, Zeke and Turner walked in and out of the lattice, like Kenan and Pascal. Observing the lattice from afar, they discussed the overall structural similarities between snowflakes and ice lattice, including the hexagonal symmetry and the branches of snowflakes. By observing the lattice from within it, they discussed that the tetrahedral unit of the ice lattice looked very uniform and would keep its uniform arrangement as the lattice grew bigger with more water molecules. But, like Kenan and Pascal, they also pointed out that certain parts of the snowflakes (e.g., variations of snowflakes' branches) cannot be explained by observation of the ice lattice.

Similar to pairs with a clear understanding of hydrogen bonding, Zeke and Turner's interaction and discussion during the simple structures were similar to the activity with magnetic models. However, the dynamic changed during complex structures. By constructing complex structures, this pair explained the 3D hexagonal arrangement in a lattice in relation to the six-fold symmetry of snowflakes. However, seemed to be overwhelmed by the complexity of the ice lattice; their diagram did not clearly show the hydrogen bond between water molecules.

4.7.6 Conceptual Understanding After iVR Activities

For the concept of hydrogen bonding, both aimed to illustrate the 3D hexagonal pattern and the "zigzag" pattern they saw in the ice lattice inside iVR. Zeke explained that he was drawing ice structures without drawing the atoms of water molecules. Thus, his understanding of hydrogen bonding cannot be fairly categorised. His drawing also looked like hydrocarbon, suggesting he was trying to find the parallel with familiar structures he encountered in his class. Turner, like Kenan, provided another drawing in addition to his previous drawing to show a top and side view of the structure. He explained that the molecules interacted through hydrogen bonding in 3D space. However, he drew the water molecules touching each other, which implied that he was still unsure about the distance between water molecules.

For the concept of snowflake formation, Zeke elaborated on the growth of the six-fold symmetry of snowflakes, starting from a single water molecule hydrogen bonded to form tetrahedral, 3D hexagonal shapes, layers, and finally, 3D hexagonal lattice. Turner also explained the relation of a hexagonal lattice with snowflakes but did not mention tetrahedral. Both added information about environmental factors related to the variation of snowflakes' branches.

4.8 Cross-Case Analysis of Students' Conceptual Changes and Interaction With Magnetic Models and Within iVR

The previous sections present the learning journey of six pairs of students to learn hydrogen bonding and snowflake formation with magnetic models and immersive virtual reality learning activities. This section presents commonalities in students' conceptual changes and interactions observed from the cross-case analysis of six pairs of students. Students' explanations of the hydrogen bonding and snowflakes' explanation before and after each activity were categorised and summarised in Tables 4.7 and 4.8.

For the concepts of hydrogen bonding, students started with various levels of understanding of hydrogen bonding. After activities with magnetic models, students generally showed an understanding of the interaction between water molecules in terms of O-H attraction between water molecules and the maximum number of hydrogen bonding per water molecule. However, the idea of distance between water molecules was not considered. Before iVR activities, students added the idea of distance and angle in their explanation of hydrogen bonding. After iVR activities, students mostly showcased interactions between multiple water molecules in 3D space, resulting in a hexagonal shape. However, some students did not clearly represent the O-H attractions between water molecules after iVR.

Table 4.7

Change in Students' Understanding of Hydrogen Bonding Based on Their Diagrams and Explanations

Student	Before magnetic models	After magnetic models	Before iVR	After iVR
Ana	Category A H-H attraction.	Category C O-H attraction. Max number of H-bond.	Category B O-H attraction at a distance, but the role of lone pairs was unclear.	Category B 3D O-H attraction, but the role of lone pairs was unclear.
Mark	Category A H-H attraction.	Category C O-H attraction. Max number of H-bond.	Category A O-H and H-H attraction.	Cannot be categorised.
Fiona	Category B Unclear role of lone pairs.	Category D 3D O-H attraction in tetrahedral.	No change from the previous.	Category D 3D O-H attraction in hexagon.

Elena	Category A O-O attraction.	Category C O-H attraction. Max number of H-bond.	Category C O-H attraction at a distance.	Category D 3D O-H attraction in hexagon.
Nigel	Category B Unclear role of lone pairs.	Category C O-H attraction. Max number of H-bond.	Category C O-H attraction at a distance and an angle.	Category D 3D O-H attraction in hexagon.
Jasper	Category B Unclear role of lone pairs.	Category A Unclear inter vs. intra bonds.	Category A Unclear inter vs. intra bonds.	Category D 3D O-H attraction in tetrahedral.
Tiana	Category C O-H attraction. Max number of H-bond.	Category C O-H attraction. Hexagon.	Category C O-H attraction at a distance and an angle.	Category A Unclear H-bond.
Renee	Category C O-H attraction. Max number of H-bond.	Category A Unclear inter vs. intra bonds.	Category C O-H attraction at a distance and an angle.	Category A Unclear H-bond.
Kenan	Category C O-H attraction. Max number of H-bond.	Category C O-H attraction. Hexagon.	Category A O-O attraction.	Category D 3D O-H attraction.
Pascal	Category C Max number of H-bond	Category D 3D O-H attraction in hexagon.	No change from the previous.	Category D 3D O-H attraction in hexagon.
Zeke	Category C Max number of H-bond.	Category D 3D O-H attraction in hexagon.	No change from the previous.	Cannot be categorised.
Turner	Category C Max number of H-bond.	Category C O-H attraction in pentagons.	Category C O-H attraction at an angle.	Category D 3D O-H attraction, but the distance was off.

Note. H-bond: hydrogen bonding.

For the concepts of snowflake formation, students were initially unsure and only focused on the flat appearance of snowflakes when explaining the shape of snowflakes. After completing activities with magnetic models, students recognised the link between microscopic and macroscopic structures. They directly matched the observed structures to explain the horizontal expansion of branches or the hexagonal shape of snowflakes. Before iVR activities, students generally did not change or became unsure about their explanation of snowflakes' formation. After iVR activities, students mostly explained the parallel between hexagonal molecular structure and the six-fold symmetry of snowflakes. They also included other aspects in their reasonings, which included three-dimensionality, scale, growth, or environmental conditions.

Table 4.8

Change in Students' Explanation of the Formation of Snowflakes

Categories		Before magnetic models	After magnetic models	Before iVR	After iVR
Tetrahedral	Tetrahedral + hex + variation				Zeke, Fiona
	Tetrahedral + variation				
	Tetrahedral + hex				Kenan
	Tetrahedral				
Hexagons	Hex symmetry (3D) + variation				Ana, Mark, Jasper, Nigel, Turner, Tiana, Renee, Pascal
	Hex symmetry (flat)	Zeke, Tiana	Zeke, Tiana, Kenan, Pascal, Turner, Renee	Tiana, Renee, Zeke, Turner	Elena
3D interactions	3D lattice + variation				
	3D interaction (no link w/ snowflakes)			Kenan, Pascal	
Focus on appearance	Appearance (variation)	Jasper, Nigel		Mark	
	Appearance (flat branches)	Kenan, Turner, Pascal, Renee	Ana, Mark, Elena, Fiona, Jasper, Nigel	Ana, Elena, Fiona, Jasper, Nigel	
Unsure	Incoherent				
	Not sure	Ana, Mark, Fiona, Elena			

4.8.1 Students' Learning Interactions and Outcomes During Activity With Magnetic Models

Pairs of students interacted with magnetic models differently based on their prior knowledge, emphasising the extent of the educational benefits of magnetic models. Table 4.9 shows the pattern of students' interactions with magnetic models.

The activity with magnetic models helped students to establish the nature of hydrogen bonding (O-H attraction) between water molecules, especially for students with an alternative understanding of hydrogen bonding (e.g., Ana-Mark). They achieved it by feeling the attraction and repulsion between the models of water molecules. By trying to tear apart O-H between and within water molecules, students with lower prior knowledge also noticed that the intermolecular forces were different from intramolecular bonds in terms of strength. However, students who initially had an unclear understanding of hydrogen bonding were still unsure of the reason for O-H attraction.

The activity with magnetic models helped students learn that O-H atoms attract, but most students represented the interaction between water molecules as almost touching each other. Seeing no gaps between magnetic models might prompt students to think that the length of hydrogen bonding or the distance between water molecules is minimal.

Students develop an appreciation of the 3D spatial arrangement of water molecules during the activities with magnetic models. By looking at the model, students recognised the location of lone pairs on oxygen atoms that are perpendicular to the hydrogen atoms of water molecules. They also learned that each of the lone pairs was capable of attracting another water molecule. This exploration of the directionality of hydrogen bonding (in terms of lone pair) was especially prominent in pairs with a partial understanding of hydrogen bonding, such as Nigel-Jasper. They spent more time exploring the maximum number of hydrogen bonding for one water molecule and discussed the resulting tetrahedral structure. Despite understanding the orientation of lone pairs and the resulting tetrahedral formation, some students did not emphasise the 3D aspect of water molecules interaction. Instead, they focused on how similar their drawings looked to the flat structure of snowflakes.

Students with higher prior knowledge (e.g., Zeke-Turner) used magnetic models to test the stability of various molecular structures and found that cyclic structures – pentagons and hexagons – were relatively stable. However, magnetic models are limited when supporting students with higher prior knowledge to explore ideas about the growth of ice lattice structures in 3D directions. After the activities with magnetic models, some of these students drew hydrogen bonding as interactions between oxygen atoms instead of O-H atoms of water molecules, while others did not show the difference between hydrogen bonding and covalent bonding. Perhaps these students too focused on capturing the cyclic formation in drawing, which resulted in unclear representations of hydrogen bonding.

Table 4.9

Students' Conceptual Explorations During the Activity With Magnetic Models

Students	Testing attraction and repulsion	Building tetrahedral structure	Building cyclic structures	Building lattice structures
Mark & Ana	Extensively to learn O-H attraction.	After being prompted.	Testing stability of linear and cyclic structures.	None.
Elena & Fiona	〃	〃	Testing stability of linear and cyclic structures. Discussed inter vs. intramolecular bonds.	None.
Jasper & Nigel	Confirms O-H attraction; molecules rotate to bond.	Extensively, to learn the max number of H-bonds for a water molecule.	Testing stability of various cyclic structures.	None.
Tiana & Renee	Confirms O-H attraction.	Confirms tetrahedral.	〃	Attempt to build but tear it apart/crumbles.
Kenan & Pascal	〃	〃	〃	〃
Zeke & Turner	〃	Not discussed.	Testing stability of linear and cyclic structures.	〃

The molecular structures that students created during the activity shaped their explanations of snowflakes. Pairs with lower prior knowledge typically spent more time with two water molecules and creating tetrahedral structures during the activity. They explained that the snowflakes' arms or branches would have resulted from the four binding regions of water molecules. In contrast, pairs with higher prior knowledge explained that six water molecules formed the hexagonal structures, and the hexagonal structures looked similar to the hexagonal shape of snowflakes. For mixed prior knowledge pairs, they explained both branching and the cyclic (not exclusively six-fold) symmetry of snowflakes. However, the link between the branching and cyclic symmetry was unclear as they had not established how the molecular structure would expand in vertical and horizontal directions.

Regarding social interactions, students with higher prior knowledge seemed more ready to talk to their peers than students with lower prior knowledge. The analysis of students' interactions showed that students mostly interacted one-on-one with the interviewer instead of with each other. While students answered the interviewer's prompts, the others listened and agreed with their peers' explanations. The individualistic interactions mostly happened with pairs with alternative prior knowledge when they explored the attraction and repulsion of the tetrahedral structure. Students with higher prior knowledge differed from others because when they created a 3D ice lattice, they combined their magnetic models and discussed their observations with each other.

4.8.2 Students' Learning Interactions and Outcomes During iVR Activity

Students showed different levels of conceptual discussion during the simple (two water molecule, tetrahedral) and complex (single layer, three layers, ice lattice vs. snowflakes) structure tasks, depending on their level of initial prior knowledge. Table 4.10 shows the summary of students' conceptual exploration. The different interactions showcased by each pair of students highlighted the different learning benefits of iVR.

Students developed an understanding of optimal orientation (angle and distance) between water molecules in iVR, especially for students with initial alternative understanding (e.g., Ana-Mark). They extensively explored the simple structures to establish the 3D orientation of O-H attractions between different water molecules. However, these students got overwhelmed by complex structure tasks, so their scientific discussions did not move beyond the description of surface features of the complex structures task. These students only focused on the salient hexagonal patterns while exploring complex structures.

Students with clear prior understanding explored more when they saw more water molecules around them during the complex structures task. Unlike their counterpart, students with higher prior knowledge still held preconceptions during their interaction in simple structure tasks, which sometimes were inappropriate to describe the interactions of water molecules in 3D (e.g., 180° as the optimal angle). However, they seemed to engage more in complex structure tasks. By manipulating, walking, and bending around the structures, students could discuss new ideas that were difficult to study with magnetic models, such as the link between tetrahedral subunits and hexagonal patterns in ice lattice. These students noticed and discussed the implications of different 3D features (e.g., subunits, chair conformation) towards the growth of 3D complex structures.

The iVR learning activity helped students understand the 3D spatial arrangement of water molecules. In general, students included wedge lines or provided multiple drawings to highlight the three-dimensionality of their drawings after iVR. When they could not draw, they explained verbally that some of the molecules they had drawn were tilted, going in and out of the page. Regardless of their prior knowledge, students were generally shown that many water molecules formed a 3D cyclic structure. Some students, especially the ones with clear prior knowledge, focused on capturing the complexity of ice structure in their drawings, including the hexagonal pattern, chair conformations, and layers of hexagons. However, while capturing these complexities, some students seemed to forgo the basic concepts of hydrogen bonding. Some students did not represent a complete structure of water molecules (H_2O) in their drawings. It was unclear how they conceptualised the O-H interactions between water molecules without drawing the structure of water molecules. These students also noted the involvement of tetrahedral formation in the creation of complex structures but were uncertain about how to articulate these interactions on paper in terms of individual water molecule interactions. Perhaps these students were choosing to focus on representing the ideas related to the complex structure because they have already demonstrated their ideas on the basics of hydrogen bonding. Another reason why students did not clearly represent O-H attraction after iVR is perhaps because students were astonished by the complexity of molecular structure in iVR and then became unsure about the basic nature of hydrogen bonding.

In terms of snowflakes' formation, iVR activities helped students explain the shape of snowflakes in terms of the six-fold symmetry. Unlike the students' explanation after the activity with magnetic models, students explained how the hexagonal structure grew in vertical and horizontal directions to form a 3D ice lattice after iVR. Students also incorporated multiple ideas in their explanation of the six-fold symmetry of snowflakes after the iVR learning activity. Most of the students explained the effect of environmental conditions on the variation of snowflake patterns/branches and symmetry. Students with a higher prior knowledge more readily provided extended explanations of snowflakes that link many ideas (three-dimensionality, scale, growth, and subunits).

In terms of social interaction, it changed depending on the task in iVR. Pairs with leader-follower dynamics maintained their behaviour during the simple structure tasks but contributed more equally when completing the complex structures. However, when students receive external hints, they tend to continue relying on hints instead of each other. Compared to their interactions during the magnetic model activity, students talked more inside iVR, perhaps due to the absence of interviewers

Table 4.10

Students' Conceptual Explorations During the iVR Activity

Students	Simple structure tasks				Complex structure tasks			
	Two molecules (Forming H-bond)	Two molecules (Angle & distance)	Tetrahedral	Two clusters	Single layers	Lattice (Subunits)	Lattice (Shape of snowflakes)	Lattice (Growth)
Mark & Ana	Extensive exploration.	Focused on colour & thickness to explain bond strength.	Not sure 4 or 2 H-bond. Formed rings.	Staggered hexagons.	Struggles (Unsuccessful).	Not discussed.	Six-fold symmetry.	Growth of lattice + randomness (Unsure).
Elena & Fiona	”	Focused on colour & thickness.	Not sure 4 or 2 H-bond.	Focused on single hexagons.	”	”	Branches.	Not discussed.
Jasper & Nigel	Formed without struggles.	Focused on angles (180°) to explain bond strength.	Predict 4 H-bond.	”	”	Discussed.	Hexagonal symmetry + branches.	Growth of layers.
Tiana & Renee	”	Focused on distance and angle (180°) to explain bond strength.	”	Staggered hexagons + hexagonal channel.	Struggles (Successful).	”	Six-fold symmetry.	Growth of hex centre + randomness.
Kenan & Pascal	”	Focused on distance and angle (0°) to explain bond strength.	”	”	Successful.	”	”	Growth of repeating units.
Zeke & Turner	”	”	Predict 4 H-bond. Formed rings.	”	”	”	”	”

Chapter 5. Students' Evaluation of Learning Experience With Magnetic Models and Within Immersive Virtual Reality

This chapter illustrates how twenty pairs of students evaluated their learning experience with magnetic models and within an immersive virtual reality (iVR) environment. Students' responses were categorised into four immersion categories (visual, interactivity, social, and narrative) and were compared. The learning focuses on the concepts of hydrogen bonding in the context of snowflake formation. This chapter is organised into three main sections.

Section 5.1 presents the results of cross-case thematic analysis of students' evaluation of learning experience with magnetic models. This section corresponds to Research Question 2a.

(a) How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation when using *magnetic models*?

Section 5.2 presents the results of cross-case thematic analysis of students' evaluation of learning experience with iVR. This section corresponds to the second part of Research Question 2b.

(b) How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation within an *immersive virtual reality* environment?

Section 5.3 summarises the comparison between students' evaluation of learning experience with magnetic models and iVR.

5.1 Students' Evaluation of Learning Experience With Magnetic Models

Most students found that the activity with magnetic models was "great" and "interesting". A few students mentioned that it was fun to "play" with the magnetic models. Students' responses were further categorised into four immersion features: interactivity, visual, social, and narrative features. The most highlighted feature of magnetic models was **interactivity** – having tactile feedback to assist students' active exploration of molecular interactions and structures (n=20 pairs). Many students (n=16 pairs) also appreciated being able to visualise molecular structures in 3D **(visualisation).** Eight pairs discussed the benefit of having a partner to bounce ideas or have a more enjoyable learning experience **(social).** However, most pairs felt the activity with magnetic models was individualistic despite the presence of their partner (n=10 pairs). In terms of **narrative**, students felt the task was engaging because of the student-driven nature and the opportunity to interrogate their prior knowledge (n=9 pairs). In the following sections, students' evaluations of the four main features are elaborated.

5.1.1 Visualisation Feature of Magnetic Models

Students appreciated being able to observe the 3D structure of water molecules with magnetic models. The majority of students (n=12 pairs) mentioned that magnetic models were particularly useful for observing tetrahedral and ring structures. In their comments, students noticed the missing 3D aspects in the structures they drew after observation of the magnetic models. With magnetic models, students appreciated the specific orientation between water molecules to result in 3D structures, such as tetrahedral, pentagons, and hexagons.

> Ella: "*Also, it helps you more if, in terms of understanding that molecules aren't 2D like they are, they're 3D, so then the different bonding will create a different shape. Yeah, it won't look like a flat diagram like this. And it looks something like that [points at the magnetic models].*"

Some students (n=4 pairs) also appreciated the visualisation of the water molecules feature. They thought the representation of water molecules as a space-filled model was useful for observing the position of lone pairs and the size difference between oxygen atoms and hydrogen atoms. Students elaborated that knowing where the lone pairs were was helpful in understanding how the water molecules would interact to form certain molecular formations. However, a few students (n=2 pairs) recognised the limitation of observing the hydrogen bonding. They reason that when the magnetic models attached to each other, it was hard to observe which ones were the hydrogen bonding and which ones were the covalent bonds.

> Luna: "*I think, like, the colours help as well because you can clearly see and feel like the oxygens are smaller. And then, sorry, I mean, the hydrogens are small.*"
>
> Stella: *"I feel like we needed the understanding of kind of how these bonds work. You can't just, like, if you gave me this, I wouldn't [understand] if I didn't have any previous understanding of intermolecular bonds. It doesn't show you the electron pairs or anything."*

5.1.2 Interactivity Feature of Magnetic Models

Students enjoyed being able to feel the attraction and repulsion between magnetic models. Students explained that the attraction and repulsion helped them to understand the atoms O-H attract and the atoms H-H and O-O repels (n=14 pairs). Three pairs specified that interacting with magnetic models clarified the difference between hydrogen bonding and covalent bond (intermolecular forces vs. intramolecular bond). They explained that the idea came from recognising that pulling apart two models of water molecules was way easier than pulling apart hydrogen atoms and oxygen atoms in models of water molecules. For a few pairs of students (n=3 pairs), the act of detaching and attaching two models of water molecules gave them ideas about putting and releasing energy during the breaking and forming of bonds.

Ella: *"[With diagrams] You just wouldn't be able to understand the bonding in them. So why, like, they're attracted to each other, right? These ones [magnetic models] help because they've got the magnets."*

Gwen: *"And like the difference between the covalent and the hydrogen bonding. Okay, that was interesting because I didn't know. I would have thought the hydrogen bond was stronger."*

In addition to the attraction and repulsion, students explained that the magnetic models helped them construct and discover tetrahedral and cyclic structures (n=12 pairs). Most of these students commented that they knew two water molecules could form a hydrogen bond. With many models of water molecules, they explained that they were surprised to see that water molecules could form different structures, such as tetrahedral, linear, pentagon, and hexagon shapes. However, some pairs (n=3 pairs) explained that it was difficult to draw conclusions about the stability of the molecular structures and decide which structures are responsible for the shape of snowflakes. These students elaborated that making a more complex structure (e.g., ice lattice) was challenging because the structure became unstable as they made it bigger.

Zeke: *"And then it's interesting just to get even more and more because then you get to learn how lots and lots of different molecules interact together and what kind of structures they can or can't form. And you can see how some of them might be more stable or less stable than others."*

Luke: *"It [magnetic models] won't do what I want it to do. So, if I want to do that, as the arrangement gets bigger, the way it bonds to itself becomes a little bit more complex. And I can't get perfect rings to join up with perfect rings because they're not symmetrical shapes. I was … what I always thought was water is a little bit more organised."*

5.1.3 Narrative Feature of Magnetic Models

Some students felt that their experience with magnetic models was engaging because of the way the task was designed. Compared to their chemistry lectures, students thought that the activity with magnetic models was more memorable and felt like a lot less work. These students appreciated having the opportunity to come up with their own conclusions instead of being told what to do. They mentioned that their brain stayed active because they had the freedom to observe, explore, and solve a "puzzle" (n=4 pairs).

> Patrick: "*I had a pretty interesting experience on played around with models or anything at one time. And what I found was when I'm learning from a lecture or something, like, my brain switches off. I find that it [magnetic models] gets me thinking a lot more. I'm observing and exploring. So, it was a very different experience. And it was enjoyable.*"

Some students talked about their experience with magnetic models in relation to the drawing task (n=5 pairs). By first drawing their hypothesis about water molecular interactions, students felt engaged in the activity with magnetic models to test their hypothesis.

> Renee: "*It was good because you could see how your first understanding can change once you understand what to do. […] and get to see how it [magnetic models] all fits together. You can see, oh, that doesn't work this way. These ones work.*"

5.1.4 Social Feature of Magnetic Models

Half of the students (n=10 pairs) perceived the activity with the magnetic models as an individual activity. These students elaborated that they had their own set of magnetic models and explored the sets themselves. They noticed that they could look at each other's actions. However, simply commenting on each other's actions was not enough for these students to perceive the activity as a collaborative activity.

> Simon: "*I feel like it's you individually. Because I was doing my own thing, and she was doing her own job.*"

Some student pairs appreciated having a partner to bounce ideas (n=6 pairs), make the activity more fun (n=2 pairs), or complete the activity faster (n=1 pair). These students realised that sometimes their partners created different structures or noticed different aspects of the molecular structures. They mentioned that the different perspectives helped them to have a more productive learning activity or to get the idea faster. Some of these pairs were strangers, while some were friends. This suggested that students' affiliations did not seem to affect their appreciation of having a partner during the activity with magnetic models.

Max: "*Yeah, like, it's definitely beneficial to have another person here to sort of do it with rather than just doing it alone. Because you can sort of, Yeah, bounce ideas off each other.*"

Ella: "*And then when I was like interacting my molecules with Alice's [her partner]. So, just like, I think that was fun. Yeah.*"

5.1.5 A Closer Look of Students' Evaluations of Learning Experience With Magnetic Models

These findings show that students' characteristics seemed to influence how they evaluate the learning experience with magnetic models. The perspectives of two pairs with different background knowledge are illustrated below.

Ana and Mark. This pair liked their experience with magnetic models. Drawing a comparison with their online workshop during the pandemic, they explained that having a hands-on activity made the abstract ideas more real (visual and interactivity features). Ana explained that she was struggling with the concepts of bonding, but by feeling the attraction and repulsion, she could understand how water molecules interacted with each other (O-H attraction). These two students also highlighted that the hands-on activity made the lesson more interesting. When asked about collaborations, these students appreciated having a partner with whom to bounce ideas (social feature).

Kenan and Pascal. This pair stated that the experience with magnetic models was nice and good because it was easy to understand, better than learning with paper. Both students highlighted the different 3D structures that they could construct, which they could not possibly do with 2D learning tools (visual feature). They explained that constructing and discovering the different structures helped them hypothesize about snowflake formation (interactivity feature). Pascal also mentioned that the activity felt like solving a puzzle, which was also echoed by Kenan (narrative feature). They appreciated having to figure out the answer themselves. This pair also appreciated having each other to bounce ideas and solve the problem faster (social feature).

As shown above, students generally highlighted visuals and interactivity as the main features in the magnetic model learning activity. Students with low prior knowledge highlighted their interactions with two water molecules to feel the attraction and repulsion, while students with higher prior knowledge appreciated the construction of various 3D structures. Prior knowledge did not seem to influence their evaluation of social features (collaboration). Regarding the narrative feature, students with higher prior knowledge perceived the activity as a puzzle or problem-solving exercise, whereas students with lower prior knowledge did not explicitly mention this aspect.

5.2 Students' Evaluation of Learning Experience Within iVR

Almost all pairs of students expressed their excitement about experiencing iVR. They used terms such as "really cool", "so fun", or "amazing". Three students (out of 40 students) reported that they felt dizzy or disoriented when wearing the headset for the first time. Despite the discomfort, these three students still explained that the overall iVR experience was enjoyable.

> Zeke: "*I don't want to sound mean because, like, it's [iVR] better than I expected. I suppose I expected something interesting, but those are actually quite fun*."
>
> Bob: "*Amazing, I loved it so much. It was just the interactiveness of it. It was just so cool.*"

When asked to elaborate on the reason why iVR was "fun" or "cool", students explained that they felt that they were in a different place – no longer in the room. They mentioned that they could only see the winter environment with snowfall around them everywhere they looked. Interacting felt intuitive, as if they were interacting with real objects in the real world. A few students mentioned collaboration with their peers made iVR a fun experience. Similar to their response in the post-magnetic model interview, students' responses in the post-iVR interviews were further categorised into four immersion categories: visualisation, interactivity, social, and narrative.

All pairs (n= 20 pairs) expressed enjoyment in visualising the 3D iVR space and molecular structures **(visualisation).** All of them were also excited to elaborate on their experience of interacting with the 3D molecules **(interactivity).** Many pairs of students (n=16 pairs) also appreciated sharing the virtual space with their peers to exchange ideas and feel more motivated to complete the learning task **(social)**. Students (n=17 pairs) also felt that the tasks were engaging in terms of the context and opportunity to apply their prior knowledge **(narrative).**

5.2.1 Visualisation Feature of iVR

Students expressed excitement about being transported to a different place. Five pairs of students highlighted that they enjoyed observing the iVR environment by mentioning how the snowfalls, the forest, or the thunder in the sky looks good and real. Students elaborated that they felt like they were "actually there" because they could only see the winter forest when they looked around. They were also amazed that 3D objects (including themselves) have shadows, which make the virtual environment feel realistic.

> Luna: "*It was amazing. [Because] we're, like, in a different climate. Yeah. And like, and we saw snowflakes.*
>
> Emily: "*I thought it was really cool. Like, I liked how, like, if you look down like, it even had like shadows and stuff. That's why I was looking [around], and I was like, whoa."*

Students appreciated being able to observe the simple (n=4 pairs) and complex structures (n=9 pairs). These students noted that it was good to see 3D water molecules in iVR because they could not see the molecules as easily in real life or other media. The majority of students pointed out that observation of complex structures (i.e., a single layer of ice and ice lattice) in iVR were unique and allowed them to appreciate the intricacies of the 3D structures, including the repeated and uniform hexagonal pattern, the zig-zag pattern, the stacked layers, and the uniform electron density areas on each side of the layer of ice.

> Emily: "*And there [iVR space], you can, like we, as he said before, like we can't actually see the molecule bond in the real world."*
>
> Gwen: "*Seeing the sheets, I didn't realise how like uniform all really was. Like, looking from that one angle, I could see the hexagons and, like, the tubes, kind of down, which is really cool. So, I think that was the biggest takeaway for me."*

Students explained that they finally appreciated the massive 3D growth after seeing the ice lattice in iVR. Even though magnetic models showed them 3D structures of hexagons, students mentioned that they could not see how the hexagons would grow in 3D directions. Unlike magnetic models, students explained that they could easily lift, rotate, or walk around the massive complex ice lattice to observe them from different angles. Students talked about noticing different aspects of molecular formation in IVR that they did not notice with magnetic models, such as the hexagonal channel. Seeing the hexagonal channel helped the students to explain snowflakes' formation after iVR.

Tiana: "*You know why we kept getting really confused [about the link between hexagons and tetrahedral]? Because we couldn't have them in 3D into layers. That's why we're getting confused here thinking before [their drawing of tetrahedral] was not correct because of that weird angle that it sets up, and you can't draw it like that."*

Two pairs of students (e.g., Rory) talked about walking around the molecular structure to observe it because they did not want to "ruin" the structure. On the other hand, two pairs of students (e.g., Stella) mentioned walking through the ice lattice to observe the "internal" arrangement of the lattice. However, they expressed the need for some time to adjust to the virtual space before they were comfortable walking through the virtual 3D objects.

Rory: "*I kept stepping around the molecule, even though I know you can walk through it. Yeah. It was just like, no, I can't touch that. It will ruin it. I need to walk around."*

Stella: "*It was a bit strange at first because it's like nothing you've ever really experienced before. But after you get used to it, it's like really interesting, because then you can, like, walk through things and like, see them kind of like put your face through the lattice is like so you can see internally and externally quite easily."*

5.2.2 Interactivity Feature of iVR

Interaction with 3D molecular structures was the highlight of students' learning experience with iVR. In their responses, students often compared the interactivity in iVR with other media they commonly used in class. They said that manipulating the molecules using their hands in iVR, such as grabbing and rotating them, was more intuitive and easier than manipulating a 3D visualisation on a 2D screen.

Marty: "*In VR, you could, like, do all directions at the same time, which is really good."*

Lily: "*It's good, like interactive. It was good that you could pick it up and turn it around like you were actually holding it as well."*

Stella: "*With VR, it was easier to manipulate in a 3D plane in a way that you understand it. Because even though on the computer it's 3D, it was still like 2D screen*."

The intuitive interaction was beneficial for the students to explore water molecules (n=11 pairs) and complex structures from different angles (n=11 pairs). Unlike magnetic models, students did not talk about feeling tactile feedback of attraction and repulsion. However, these students explained that interacting with molecules felt like they were "touching" real molecules even though they were aware that they were manipulating a virtual 3D object in iVR. Student elaborated that the way they were able to easily interact with the molecules in 3D space made them forget that they were dealing with virtual objects and continue to perceive the virtual objects as "real".

Kimi: "*It's like you're not in reality. But you're … it's like close, yeah, virtual reality, as the name suggests. You can position it in a way you can play with molecules, like in real time and space.*"

Bob: "*You sort of forget that it's not there like it's not real? It's, like, actually there.*"

However, two pairs of students explicitly mentioned that they were missing the tactile feedback in iVR, which made the interaction feel a bit unnatural.

Zeke: "*Like that [magnetic models], you can really feel it and touch it and grab it, and you can really feel it. That one [iVR], you can sort of feel it, touch it, grab it, but you are still a little bit disconnected in a way.*"

Patrick: "*I experienced a little bit of disorientation, not because of how I felt but like yeah, like you grab the onto the molecules or whatever. And they're weightless.*"

In the iVR space, students walked around to reach molecules that were located far away or to get a different view. Students explained that standing and walking around during iVR activity made learning more enjoyable. Although they could not see the real space, students talked about being aware of the location of the walls and objects in real space (n=12 pairs). The awareness of the real space usually lasts for the first few tasks. Students explained that they tended to be cautious of their movement while still being aware of the real space.

Stella: "*Yeah, because I didn't want to hit the wall because I was still aware, essentially, the grid that there was like a wall and a boundary.*"

Students appreciated being able to construct various 3D molecular structures in iVR. They (n=8 pairs) highlighted the benefit of experimenting with the angle and distance when forming hydrogen bonding. They recognised that the colour and the thickness of hydrogen bonding changed depending on the orientations of the two water molecules with each other. Students felt that being able to adjust the position of the water molecules and see an instance of visual feedback (colour and thickness) helped them to deduce how the angle and distance between molecules affect the hydrogen bond strength.

Ana: "*So, like, you know, it was very visual having to create, you know, the hydrogen bonds, when it's like that red colour, and it's yellow, and it's green, then you can* *move it just the tiniest bit and the bond snaps, and it goes away. It's a very good way to understand how bonds work."*

Students compared the activity to form hydrogen bonding in magnetic models and iVR. With magnetic models, students appreciated being able to visualise the angle between two molecules but not the distance. Unlike with iVR, students elaborated that observation of the range of angles and distance was difficult with magnetic models because as the models got close, they automatically snapped into one optimal orientation. These students realised the subtleties of spatial arrangements between two water molecules after iVR.

Marty: "*I can't really understand angle and distance with this [magnetic models] because it only snaps on one angle, and like, you can rotate it as well. And, like, there's no distance factor, and this just sticks to it. […] And then when it goes into VR, you get like, you know, real understanding, like how fine the angle is."*

Half of the student pairs appreciated the opportunity to construct complex structures (n=10 pairs). These students explained their thinking process when constructing a single layer of ice. Most of them started with mix and match for a while until they successfully connected a few clusters of molecules. Then, they stepped back and found a pattern that could become a clue to complete the structures. Most of them talked about the zig-zag pattern (when viewing the structure from the side) as the key clue. Students also highlighted that constructing complex structures without guidance helped them develop their problem-solving skills.

Owen: "*Yeah, well, while putting the three clusters to make it work together. I saw the cage pattern or some sort of shape like that. I think it was a nice problem-solving."*

On the other hand, some pairs (n=10 pairs) viewed the interactivity opportunity to construct complex structures as a bit overwhelming. They wished for more guidance to construct the complex structures successfully. These students explained that they already performed the correct strategy to construct the structure, which was making sure the hydrogen bonding was strong (thick and green). They could not figure out why the clusters of water molecules were still blinking – a sign that the cluster was still not properly aligned and connected. These students wished that the researchers would intervene and provide more hints on the next steps they must take to construct complex structures.

Ruth: "*It was confusing [constructing the single layer of ice]. I think because we tried to in different ways, and we're just like, why is it not working? Yeah. Right. So, then we just go to the [next task].*"

Among the ten pairs of students who discussed their struggles when building complex structures, half of them successfully constructed a single layer of ice. After looking into students' backgrounds, including their prior knowledge and their interaction during the iVR session, we found interesting patterns of group dynamics. Most student pairs who expressed struggles and did not successfully construct the single layer had lower prior knowledge of hydrogen bonding. Even though they showed collaborative social dynamics by taking turns in manipulating the 3D objects and building on each other's ideas, these students' limited prior knowledge might hamper them in constructing complex structures. Student pairs who successfully constructed the single layer despite being frustrated had a better understanding of hydrogen bonding. However, they were more individualistic in terms of their spatial and social interaction in iVR.

In terms of constructing complex structures, students also talked about building structures, such as an ice lattice, that they could not construct with magnetic models. Students explained that magnetic models were useful as a starting point to learn basic ideas before applying them to constructing complex structures in iVR. Unlike magnetic models, students explained that they could interact with many more molecules and easily join them to build bigger structures. Students added that being able to construct complex structures was beneficial to their problem-solving skills and to recognise the link between microscopic and macroscopic levels.

Max: "*Like little magnets were unstable when you put too many of them together. But I think it said we had 150 water molecules in there [iVR]. And we had, like, 12 here [magnetic models]. So yeah, it would have been impossible with these [magnetic models] to actually be able to properly look at the lattice structure and how that exponentially forms outwards into snowflakes.*"

5.2.3 Narrative Features of iVR

Students highlighted that they were more engaged or more focused on the task in iVR compared to their previous experience with other learning media or in the classroom. Students (n=7 pairs) felt satisfied being able to polish their problem-solving skills or analytical skills in iVR. They appreciated the freedom they had in figuring out solutions to a new and challenging task in iVR. Students mentioned the interactive feature as one of the factors that made them appreciate the problem-solving aspect of iVR.

Lucas: "*Yeah. I think it improves my analytical problem-solving skills. Yeah. Because when I answered questions, I just went with easier questions. But with this [iVR], I can be more analytical, like, more detailed in finding it."*

Stella: "*And it's also like a really immersive experience. Yeah, it's like really interactive, and it's almost kind of like a game, trying to solve it."*

Students appreciated the task design, which allowed them to build their knowledge. Five pairs of students mentioned that completing the task from simple towards complex structures was informative and helpful for their learning. They pointed out that the student-driven stepwise task helped them to make connections between the concepts they discovered in each task. They predicted that without the stepwise task, they would be overwhelmed with the complexity of concepts in later tasks (e.g., ice lattice vs. snowflakes task). Students also considered the iVR activity helpful in consolidating or applying their prior knowledge (n=13 pairs). They also considered their learning progressions from previous media in helping to construct knowledge in iVR. Students explained that the basic concepts that they had learned with magnetic models were the building blocks, and iVR was a good place to bring all those building blocks together. One pair explicitly mentioned that the concepts discussed during the iVR activity were relevant to their course.

Ana: "*I really thought everything, like the way I like to the baby steps of it, and then you put it together and then like, bigger, bigger, bigger. […] It's memorable in the sense that it walks you through it instead of just going with assumed knowledge."*

Max: "*I think they're a necessary building block. Yeah, it's definitely there are definitely benefits to having a progression of knowledge working up to it, rather than just having only VR without other resources to draw off. Yeah. Because we sort of went in steps of two-dimensional and then three-dimensional, one, four-dimensional [laughs]."*

Compared to post-magnetic model interviews, more students talked about having control over constructing their knowledge (five pairs after magnetic models vs. 17 pairs after iVR). This is perhaps because, in iVR, students' exploration was not facilitated by an interviewer like during the activity with magnetic models. Students perceived that they learned better when they could discover the solution themselves instead of being told the correct answer.

Kevin: "*We could definitely be more focused without any help. We can create more questions for ourselves. And yeah, that definitely helped us go to many hypotheses that we're thinking [about].*"

5.2.4 Social Feature of iVR

The majority of students showed a positive response regarding experiencing iVR with another student. When asked why they appreciate having a partner in iVR, students provided reasons related to conceptual aspects or emotional aspects. Only one pair of students explicitly mentioned that they preferred to complete the iVR experience alone. Sharing the virtual space with another person was a new experience for all of the students. Previous experiences students had with iVR included solo games or solo 360-degree videos. In the post-iVR interview, students also talked about how they communicated with their peers inside iVR and how they navigated between real and virtual spaces.

Compared to activity with magnetic models, more students appreciated having a partner in iVR. Students (n=10 pairs) explained that they had their own models, came up with their own ideas, and felt a bit disconnected from their partners during the activity with magnetic models. In contrast, more students (n= 16 pairs) saw the benefit of having a partner in iVR. They explained that they were sharing the task with their peer, specifically when they constructed the structures together and discussed what they noticed with their partner. Students also mentioned that having a common goal was helpful to better collaborate with their peers.

Nigel*: "Because with the models, it's just a single piece with each other. Single, like you have your own, and you're building it up. And obviously, the only collaboration is you talking to each other about what you're going to do. [In iVR] You're both using the same thing and physically interacting with it. Yeah, while also getting that somewhat specific part with it. And you know, like working together to build something, so yeah, really good. I've enjoyed it."*

Being able to bounce ideas was the main reason for students (n=12 pairs) to say having a partner in iVR was a good experience. These students recognised that sometimes they were stuck when trying to make sense of the task in iVR. Therefore, these students felt that having a partner go through the same task with them helped them get different ideas and come up with a solution for the task. Some students explained that when they were talking to their peers, they first had to organise their own thoughts and highlight important information. In this way, students found that externalising their ideas helped them to learn better compared to simply listening to information or receiving guidance from the researchers.

Logan: "*They can explain it to you a lot easier than you just trying to figure it out. They can help you along the way. And vice versa as well. So, it's like constructive learning.*"

Ana: "*If you were alone, I don't think you have that same level of thinking. Because there's like speaking out loud, having someone to bounce ideas off of and hearing other people's thoughts then helps you come to your own conclusions.*"

For some students, having a partner made the iVR experience more enjoyable (n=9 pairs) or faster (n=1 pair). In comparison, only two pairs of students talked about having fun during the activity with magnetic models. Students mentioned that it was fun to have their peers in iVR because they could motivate each other to complete the task. They commented that if they were to do the experience alone, it would be "boring" or "annoying". Some students also mentioned that it was good to "share the suffering" with their partner, which drove them to keep going with the task. Most of these comments referred to their experience of making complex structures.

Renee: "*Yeah. I think it probably might be a bit boring doing it by yourself. Oh, yeah. Because it's that much going, you just be like, oh, let's move this stuff there and there. […] Yeah. Like it was just yourself, (you would say) ah, this doesn't really matter.*"

Tiana: "*Two brains work better than one. Solving problems double the speed.*"

A few pairs of students (n= 3 pairs) appreciated the presence of their partner because they made the iVR experience more comfortable. These students were most likely aware of the presence of the researchers observing them, even though they could not see the researchers inside the iVR space. Students realised that they might look and act strange in the observers' eyes. However, having a partner share the same experience helped students to be less cautious of observers' judgement and more immersed in the iVR tasks.

Marty: "*And also, like when you have the headset on, like, you know, you always feel like a little bit dorky when you're just like swinging around wildly, but like if there's someone there with you, like, it feels less awkward because, like you're both doing it. And you get into it a bit more, I think.*"

Abby: "*(It was good to have a partner) Yeah. It's going to be so awkward talking to yourself.*"

One pair of students (Carter and Rob) started the conversation about collaboration on a positive note. They commented that the collaboration was better during the iVR activity than during the learning activity with magnetic models. It was better because they could share the workload more easily than continuously taking turns in previous activities. However, both students preferred to complete the iVR experience alone. Rob explained that he needed time to organise and externalise his ideas to his peers. On the other hand, Carter discussed his need to complete the task as fast as possible. Carter also regarded that some of the tasks in iVR were simple enough for him to complete without support from another student, except for the task of constructing a single layer of ice. Perhaps the mismatch of students' learning approaches, with Rob taking time and Carter being fast, made them think that it could be better to complete the task individually.

Rob: "*I seem to like, understand something, and then it'll take me a period of time. I don't really understand how to explain it. It's like, I can't explain what I'm thinking to people until I've already figured out what I'm thinking about.*"

Carter: "*It's always something that's, like, more efficient to just Google it. But with harder concepts, like group work like that, it's always more efficient for me because I learn a lot quicker in a group setting. But, you know, for smaller stuff. I think it's more efficient to do it individually.*"

In this study, students were represented as an *avatar* in the form of a floating grey head without facial expression and two pink hands. Most students adapted to this different embodiment by using alternative modes to communicate, while few others felt that the avatars were hindering their social interaction. The topic of *communication with peers* only emerged in post-iVR interviews because students perceived the avatar as a different way of communication. In contrast, the mode of communication during activity with magnetic models was not too much different from their chemistry classes or everyday life.

Students found no issue communicating with their peers in the iVR space (n=11 pairs). Students mentioned that they could still recognise their peers' expressions through talking and intonation of their voices. They explained gestures facilitated their interactions in iVR. These students explained that the avatar also helped them to know where their partner was inside the iVR space. Knowing their partner's position helped them navigate the space safely, including where to walk and move their hands. Students also explained that having the avatars – a 3D representation of their bodies – was important to promote and maintain social interaction. For example, they turned around and looked at the avatars when engaged in discussions. Even though the avatar did not have facial features of expression, these students still perceived "eye contact" or "a slight smile" when looking at their peer's avatar.

Jasper: "*But every time Nigel talked, I looked at that avatar. Yeah, I wanted to engage because I had something there. I felt like I was engaging with it. If it was just a voice, I don't think I would have got that same experience."*

Mark: "*(iVR is different from an online meeting) I think it's because it's 2D. I don't know. Because, like, I think it's an actual fact that I could turn around, and you're there. You could be sitting in a room in Switzerland."*

One student (Emma) also highlighted that she enjoyed talking inside iVR. Her partner, Simon, pointed out that she talked more during the iVR activity compared to during the previous activity with magnetic models. Emma explained that she could see the researcher in previous activities with other media. Meanwhile, in iVR, she could only see her partner. She said, "I kind of like talking when I don't see people". But she has no problem with the avatars and still recognises Simon's presence. She commented, "Because I did not feel like I was there by myself while I was there". Perhaps not being able to see other people's facial expressions empowered Emma to talk more and engage in the learning task.

Three pairs of students talked about social isolation inside iVR due to being unable to see their partners' facial expressions. These students acknowledged that the avatars indicated where their peers were inside the iVR space. However, they explained that the avatars were not enough to truly represent their peers in iVR. They wished they could see more representation of their peers, including their eyes, ears, arms, bodies, and legs. Without the visual indication of their peers' identities, these students felt that their social connections were hindered inside the iVR space.

Patrick: "*I found it a little bit weird. Like, you've got a sense of where the other person is because of the headset and the hands. But it's like, it's like, you lose a lot, just from the avatars, like, the avatars themselves aren't like, I don't know. You know, it's not like a real person. You don't get any like, like a sense of them."*

Simon: "*Yeah. I think so. Yeah. Because in VR, you feel isolated. Like, there's no one."*

About half of the students knew they existed in two spaces simultaneously: the real space (the room with the researchers) and the virtual space. Students discussed that they felt the presence of the researchers outside the iVR space (n=11 pairs). Students shared their feelings of being “daunted”, “cautious”, or “weird” when they were aware that the researchers were watching them. Some students elaborated that they coped with those feelings because they had their partner in iVR to emotionally support them.

Elena: “*I don’t know. Because, like, obviously like, I knew you guys were there, and I knew I looked stupid. But like, oh, just I don’t know.”*

Kevin: “And sometimes, I find it awkward. Like there, it was just us, but there were like four people in the room. And, like, is there a ghost in the room?”

5.2.5 A Closer Look of Students’ Evaluations of Learning Experience Within iVR

Similar to the evaluation of students’ experience with magnetic models, students also held different perceptions of iVR activity depending on their background knowledge. The perspectives of Ana-Mark and Kenan-Pascal are detailed below.

Ana and Mark. Neither student had experienced iVR before and had lower prior knowledge. Mark expressed excitement, attributing it to the new experience of walking around and moving 3D objects in a virtual space. In contrast, Ana initially experienced dizziness but found the interaction with water molecules in iVR enjoyable once she got used to moving around. This showed the novelty effect experienced by these two students. Both valued the ease of interaction through their 3D avatars (moving and pointing at the same object), explaining that it fostered a sense of sharing the same virtual space, enhancing collaboration (interactivity and collaboration features). Ana and Mark explained that visualising the 3D structures was helpful for their learning. They appreciated the construction of hydrogen bonding between two water molecules but expressed confusion about the construction of more complex structures, such as a single layer of ice. For them, complex structures were good to observe from different angles (visualisation feature). Constructing the complex structures was too difficult, and they wished they had more hints (narrative feature).

Kenan and Pascal. Kenan and Pascal had tried iVR before and had higher prior knowledge. They explained that their experience with iVR in this study was really good because they could move the 3D objects and observe them from different angles easily (visualisation and interactivity features). When talking about the visualisation in iVR, unlike Ana-Mark, this pair highlights the intricacies of 3D complex structures. For example, they explained how the water molecules were oriented in a single layer of ice and how the multiple sheets interacted to form a 3D ice lattice. Both appreciated that iVR gave them opportunities to experiment with different 3D spatial arrangements of water molecules to solve a problem and consolidate their learnings (narrative feature). This pair deemed having a partner helpful in their attempt to construct and discuss the 3D structures (social features).

In summary, students emphasised not only the visual and interactivity features of iVR but also the narrative and social features. Student pairs with lower prior knowledge highlighted their exploration of hydrogen bonding but found tasks involving complex structures confusing, preferring observation over construction. In contrast, students with higher prior knowledge perceived iVR as a platform for experimenting with 3D spatial arrangement – something that they could not do with other media. They welcomed the challenge and felt that the activity helped them consolidate their understanding. This showed that the narrative feature was perceived differently depending on students' background knowledge. In terms of collaboration, students generally appreciated having a partner with whom to bounce ideas.

5.3 Comparison Between Students' Evaluation of Learning Experience With Magnetic Models and Within iVR

Students generally expressed enjoyment about their learning experience with magnetic models and iVR. Their responses were categorised into four immersion categories: visual, interactivity, social, and narrative. Most of the student pairs pointed out the technological aspect in terms of observation **(visual)** and intuitive manipulation **(interactivity)** of 3D molecular structures for both magnetic models and iVR. However, students explained that observation and manipulation of 3D objects with magnetic models were different from iVR in relation to the tactile feedback and the complexity of the structures. In terms of pedagogical aspects, more students were appreciative of their partner **(social)** and became more engaged during conceptual tasks **(narrative)** in iVR compared to during the activity with magnetic models.

Students perceived learning activity with magnetic models as good because of the active play to feel attraction/repulsion and to construct tetrahedral and various ring structures. However, students felt that magnetic models were limited to exploring ideas about the growth of ice lattice structures in 3D directions. The magnetic models were also engaging because students had the opportunity to test hypotheses and improve their previous understanding. However, most students perceived the activity with magnetic models as an individual activity instead of a collaborative one.

Table 5.1

Students' Perceptions of Magnetic Models and iVR

	Key features	Magnetic models	iVR
Visual	Observation of 3D molecular structures	16	20
Interactivity	Intuitive manipulation of molecules	20	20
Narrative	Engagement in learning tasks	9	17
Social	Appreciation of having a partner	8	16

Note. N= number of pairs.

Students showed excitement when evaluating their learning experience with iVR. They highlighted the intuitive interactions with simple and especially with complex 3D structures to observe the structures from different angles. Compared to the activity with magnetic models, more students saw the benefit of collaborating with peers inside iVR to advance their chemistry knowledge. Unlike magnetic models, the communication aspect was highlighted due to the novel way of interacting in virtual space through avatars. Students also appreciated the challenging tasks they encountered in iVR as opportunities to develop problem-solving skills and apply their prior knowledge from simple ideas to more complex concepts. However, not all appreciate the challenging tasks in iVR. Students, especially those with limited prior knowledge, wished for more support in completing the challenge in iVR. These students showed more preference for exploring the intricacies of 3D molecular structures without necessarily participating in constructing them.

Chapter 6. Discussion - Students' Learning and Experience With Magnetic Models and Within Immersive Virtual Reality

Immersive virtual reality (iVR), with its advanced 3D visualisation, holds the potential to help students learn science concepts. However, most studies reported the positive effect of iVR in increasing learning engagement (Matovu et al., 2022) rather than reporting learning outcomes. For conceptual changes, most iVR studies showed an increased ability to recall information, but for higher-order skills, the benefit of iVR remained unclear (Hamilton et al., 2020). Although useful to understand how iVR supported students, the learning interactions during iVR activity were usually not reported. Students' perceptions gave an insight into the perceived usability of iVR in general (Radianti et al., 2020), but which specific aspects of iVR contributed to their learning was often unclear.

This study evaluated students' interactions, conceptual changes, and perceptions of their experience to better understand the unique educational benefits of iVR. The evidence presented in Chapters 4 and 5 will be discussed in this chapter to show the common and distinct benefits of each learning medium for students. The influence of prior knowledge and group composition identified in this study is also discussed in relation to how students interacted with magnetic models and iVR. This chapter answers the overarching question of this study:

> "What are the educational potentials of immersive virtual reality (iVR) for first-year students' chemistry learning compared to magnetic models?"

This chapter comprises three main sections: Section 6.1 – Evaluation of students' learning and experience with magnetic models, Section 6.2 – Evaluation of students' learning and experience in iVR, and Section 6.3 – Addressing challenges in chemistry learning with magnetic models and in iVR. The first two sections discuss the findings in relation to Research Question 1, which is about students' interaction and conceptual changes during the activity with the medium, and Research Question 2, which is about students' perceptions of their experience with the medium. Finally, the chapter ends with a discussion about how the findings can be used to help students overcome challenges in learning chemistry with the medium.

6.1 Evaluation of Students' Learning and Experience With Magnetic Models

Physical ball-and-stick models have been used to help students learn 3D molecular structures. Although tactile and convenient, conventional physical models were incapable of showing molecular interactions (Stieff et al., 2005). This study found that pairs of students developed their understanding of hydrogen bonding by interacting with magnetic models of water molecules. Depending on the prior knowledge and the composition of the pair, students benefitted differently in terms of their conceptual understanding of the activity with magnetic models (See section 4.8.1). Students generally perceived the activity with magnetic models as a hands-on individual activity to explore the attraction and repulsion between water molecules (See section 5.1).

6.1.1 Students' Interactions for Learning Hydrogen Bonding

Chapter 4 presented the different learning paths of six cases (pairs of students) in response to Research Question 1(a): "How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions when using *magnetic models*?"

Influence of Prior Knowledge. The findings suggest that the prior knowledge of student pairs played a role in determining how they interact with magnetic models. In magnetic models, student pairs with higher prior knowledge of hydrogen bonding created more complex structures to find the reasons for snowflake formation (e.g., Kenan-Pascal in section 4.6.2), while student pairs with limited prior knowledge explored a simpler structure to revise their understanding of hydrogen bonding (e.g., Ana-Mark in section 4.2.2). Previous studies with physical models did not report the influence of prior knowledge because the tasks typically involved observing the models instead of constructing them (e.g., Al-Balushi & Al-Hajri, 2014). Constructing structures with models engaged students' prior knowledge in a manner akin to when students created their own representation (e.g., drawing) (Ainsworth et al., 2020). In constructing their own representations, students have to organise their own thoughts and select the appropriate ideas to explore with the models. Consequently, students with similar levels of knowledge were more likely to explore the models in a similar manner.

Interestingly, the findings seemed to suggest that pairs with limited prior knowledge had more knowledge gains about hydrogen bonding by interacting with magnetic models (See section 4.8). For example, in terms of the concept of hydrogen bonding, pairs of students with limited prior knowledge seemed to make a bigger jump (from Category A to C) compared to pairs of students with higher prior knowledge (from Category C to D) after the activity with magnetic models (see Table 4.7). Previous research also showed similar findings about students with lower prior knowledge achieved higher knowledge gains than their peers with higher prior knowledge (Cordova et al., 2014). This is because the pairs with high prior knowledge already have the basic core knowledge offered by the learning task (Simonsmeier et al., 2021). Previous research suggested that more knowledgeable students performed better in more complex or demanding tasks (Kalyuga, 2007). In relation to this study, pairs with higher prior knowledge exhibited less change in their ideas of hydrogen bonding compared to the pairs with alternative prior knowledge, perhaps because the magnetic models were limited in allowing exploration of more unfamiliar complex structures by the pairs with higher prior knowledge.

Interacting With Magnetic Models. Students used magnetic models to feel the attraction and repulsion. By allowing manipulation and feeling the magnetic attraction and repulsion, magnetic models provide memorable learning experiences for students in this study, especially for the concepts of molecular interactions. Conventional physical models highlight structural arrangements but do not accommodate the exploration of molecular interactions (Warfa et al., 2014). Previous studies have used magnets and showed positive outcomes in students' understanding of electrostatic attractions (Gabel et al., 1992). For example, students could better understand the dissolution process of ionic compounds in water using magnets (Ryan & Herrington, 2014). However, because those earlier studies used flat magnets, students' explanations revolved around particulate interactions on a 2D plane. Conversely, magnetic models supported the learning of molecular interactions on a 3D plane (Warfa et al., 2014). Adding haptic feedback during the exploration of 3D structures helped students recognise the intricacies of 3D spatial arrangements that might be noticed otherwise (See sections 4.4.2 and 4.6.2). As also shown in Schönborn et al. (2011), students who have haptic feedback were more accurate in predicting the 3D orientation of protein in a biomolecular docking site.

Students pulled apart oxygen and hydrogen atoms within and between magnetic models of water molecules. Such actions helped students distinguish inter and intramolecular bonds, as shown in this study (See section 4.3.2). Modified physical models with Velcro have been used to emulate intermolecular forces and could also be used to differentiate hydrogen and covalent bonds (Schultz, 2005). Physical models can be covered with Velcro in varying strengths to help students determine different types of intermolecular forces, But unlike Velcro-modified models, magnetic models did not wear off after several times of usage (Bromfield Lee & Beggs, 2021).

Students interacted with many magnetic models of water molecules instead of just one or two, which provided them with more opportunities to observe various 3D molecular structures. Limited studies have used many physical models to learn the structures and interactions between molecules (Warfa et al., 2014). Other studies mostly focused on a single molecule, which was particularly helpful for molecules with many atoms that were difficult to represent in 2D, such as chiral molecules or complex biomolecular molecules (Bain et al., 2006). In the context of water molecules, most students were familiar with the structure of water molecules, but they were surprised to discover that many water molecules can interact with each other in linear, tetrahedral, and hexagonal formations. In chemistry lessons, molecular interactions were mainly introduced as interactions between two molecules instead of interactions of multiple molecules (Bucat & Mocerino, 2009). The activity with magnetic models in this study gave students more insight into the impact of hydrogen bonding on the 3D arrangement of molecules. Exploring the interaction of many molecules helped students to make a direct relationship between molecular structure and the physical and chemical properties of a compound (Stieff et al., 2005). As shown in this study, students made a link between the hexagonal molecular structure and the six-fold symmetry of snowflakes (See sections 4.5.2, 4.6.2, and 4.7.2).

With many magnetic models, students constructed various molecular structures and experimented with their stability. Concepts of stability of molecular structures are important for students to understand the properties of chemical compounds, for example, why diamonds are strong but graphite is not (Stieff et al., 2005). Velcro-modified models have been used to approach the idea of molecular structure stability in ice (Schultz, 2005). However, the Velcro's attraction was too strong to be overcome by gentle shakes. In contrast, molecular structures formed by magnetic models can be disrupted by shaking them. By testing which structures are more easily broken by shaking, students could reason that a chain structure is weaker than a ring structure and, thus, less likely to be found in solid-like ice. However, magnetic models are limited to assist students' exploration of the stability of bigger lattice structures. Without a specific prompt, constructing a stable lattice with a repeated uniform pattern using the magnetic models was difficult. The results showed that seeing the crumbling of lattice structures kept students developing reasoning about molecular growth in 3D directions (See sections 4.5.2 and 4.6.2).

Interacting With People. This study found that students tend to interact with the interviewer more than with their peers during the activity with magnetic models (See section 4.8.1). Previous studies suggested that students tend to rely on authoritative sources (e.g., their lectures) as the basis for their learning instead of considering their peer's ideas (Hübscher-Younger & Narayanan, 2003). Although the interviewer in this study only acted as a facilitator, the students might perceive the interviewer as an authoritative source, which prompted them to provide the "correct" answer instead of freely exploring different ideas with their peers. The effect of authoritative sources could be lessened to improve peer-to-peer collaboration by hiding the identity of the authoritative figure through technology (e.g., Hübscher-Younger & Narayanan, 2003). However, some students may not effectively collaborate without a facilitator or some form of scaffolding (Webb, 2013). As observed in this study, students needed to be prompted to externalise their thoughts and initiate discussions (See section 4.2.2). Perhaps the prompts could be given through some other forms, like paper-based or technology-enhanced text (Rau et al., 2017), to help students collaborate without hindrance from a perceived authoritative source.

6.1.2 Students' Perceptions: Individualistic Hands-On Activity

Chapter 5 (section 5.1) presented students' perceptions of their experience with magnetic models in response to Research Question 2(a): "How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation when using *magnetic models*?"

The majority of student pairs in this study perceived the activity with magnetic models as a good or interesting tactile activity to visualise and learn about interactions between water molecules (See sections 5.1.1 and 5.1.2). Students recognised that physical models helped them better visualise the 3D arrangement of molecules, as shown in many studies (Stieff et al., 2005; Stull et al., 2013). What surprised students was the tactile feedback from the attraction and repulsion between water molecules, which was memorable for them. Although no studies reported that students' perception of magnetic models was found, a similar study showed that the use of haptic feedback increased students' positive attitudes toward learning chemical bonds (Ucar et al., 2016).

A small number of students in this study reported how they appreciated the opportunity to test their prior knowledge and come up with their own understanding instead of being told what to do (See section 5.1.3). When students had an intrinsic motivation to solve a task, they were more likely to engage in inquiry or a deep learning approach, which was characterised by generating more questions and ideas and giving more elaborate scientific explanations (Chin & Brown, 2000). Students in this study mentioned that drawing about what they knew before the magnetic model task helped them engage in the task. Corroborating Ainsworth and Scheiter (2021), the findings of this study suggest that drawing before using the activity promoted the purposeful use of the magnetic models for interrogating their prior knowledge. By generating diagrams, students organised their prior knowledge and were then able to recognise the extent of their knowledge, including the misconceptions or gaps (Cooper et al., 2017b). As shown in this study, incorporating narrative features (externalising prior knowledge through drawing) before the activities with magnetic models allows students to engage in purposeful learning with the models.

Despite going through the activities with magnetic models together, most students in this study perceived the magnetic model activity as an individual activity (See section 5.1.4). These students' perceptions were in line with our observations that suggest placing students together does not always lead to collaboration. Although students reported that they were aware of each other's actions, they felt that they needed to do more than that to collaborate. Students explained that because they were focusing on their own magnetic models and drawings, they felt the whole activity was an individual activity. This study found that students engaged in productive scientific discussions when they shared their models. Collaboration can be fostered by allowing students to share tasks and easily communicate with each other (Hübscher-Younger & Narayanan, 2003). As also shown in Liu et al. (2021), by having equal control of the visualisation tool, students showed increased social engagement to build joint understanding. However, because most students in this study tend to explore their own set of models without sharing them, the opportunity to ask each other questions was limited. Promoting students to share the physical models, as shown by Rau et al. (2017), could potentially enhance social interactions and richer scientific discussion between students.

6.2 Evaluation of Students' Learning and Experience in iVR

In chemistry, iVR supports students' exploration of 3D molecular structures or provides a safe space to perform chemical experiments (Fombona-Pascual et al., 2022). Previous evaluations of iVR showed an increased student learning engagement, but learning outcomes beyond information recall were rarely reported (Hamilton et al., 2020). This study found that by interacting in iVR, pairs of students developed their understanding of the 3D spatial arrangement of water molecules in the context of snowflakes. Depending on the prior knowledge and the composition of the pair, students engaged in different tasks in iVR, which resulted in differential levels of explanation of snowflake formation (See section 4.8.2). In general, students perceived the iVR activity as a collaborative explorative or problem-solving activity to consolidate their understanding of hydrogen bonding in bigger context (See section 5.2).

6.2.1 Students' Interactions for Learning Hydrogen Bonding in Snowflakes

Chapter 4 also presented the different learning paths of six cases (pairs of students) in response to Research Question 1(b): "How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions within an *immersive virtual reality* environment?"

Influence of Prior Knowledge. In an iVR environment, student pairs with higher prior knowledge of hydrogen bonding engaged in tasks involving complex structures, while student pairs with limited prior knowledge benefitted more from simpler structures tasks. Kozma and Russell (1997) also showed that people with different background knowledge used chemistry visualisation tools differently – where experts were more comfortable generating ideas from multiple representations than novices. The analysis showed that pairs with higher prior knowledge were likely to notice various features at different levels (e.g., details of O-H bonds and the overall hexagonal channels) when constructing and observing the ice lattice. This is perhaps why these students were more successful in constructing the lattice and explaining snowflake formation (e.g., Zeke-Turner in section 4.7.5). Similar studies about chemistry visualisation tools showed that students with high prior knowledge transitioned more frequently to molecular representations to develop their conceptual understanding of relevant features (Cook et al., 2008). In contrast, students with limited prior knowledge in this study focused on one aspect of the ice lattice (mostly the hexagonal shape) and struggled to link other ideas (e.g., tetrahedral subunit). Similar observations of the tendency of students with limited prior knowledge to focus on surface features instead of relevant thematic features have been reported in previous studies (Cook et al., 2008; Kozma, 2020).

Interestingly, students with limited prior knowledge engaged and enjoyed completing the simple structure tasks, such as creating hydrogen bonds with two water molecules (See sections 4.2.5 and 4.3.5). Students with higher prior knowledge did not explore as much and tended to directly apply their preconceptions in the simple structure task (See section 4.5.5). In this study, the first couple of tasks in iVR were similar to the ones in activities with magnetic models. However, some of the preconceptions were not appropriate to explain the orientation of molecules in a 3D space (e.g., 180° as the optimal angle by Tiana-Renee in section 4.5.4). This observation about perceptual bias by higher prior knowledge was also reported by Lewandowsky and Kirsner (2000). In their study, experts tend to make errors in predicting the direction of bushfires because they focused on variables they had encountered before and disregarded new anomaly variables. This suggests that students with higher prior knowledge tend to pay selective attention in familiar situations, which could prevent them from learning something new and provide different scientific explanations (Simonsmeier et al., 2021).

Interacting Within an iVR Environment. Students intuitively grabbed, rotated, and walked around virtual 3D structures to observe them from different angles. Unlike magnetic models, students in this study experimented with the 3D orientation of molecules (angle and distance) and directly observed its implications towards the strength of hydrogen bonds. Receiving instant feedback from their direct manipulation of reified abstract concepts can assist students in testing and expanding their ideas about natural phenomena (Hennessy et al., 2007). In previous iVR studies in chemistry, students typically observed molecules in relation to the concepts of bonding (Fujiwara et al., 2020) or stereochemistry (Elford et al., 2021) without engaging in any experiment. Observation to improve understanding of the spatial arrangement of simple 3D molecules could be done equally effectively with physical models (Stull et al., 2013; Stull & Hegarty, 2016). The finding of this study suggests that unless an extra layer of information (e.g., electron density map or details about bond orientation) was included for students' experiment, showing just a simple structure in iVR may seem excessive.

Students' exploration of iVR space became more extensive as they were dealing with more complex structures (from two water molecules to a lattice structure with 150 water molecules). A limited number of studies allowed the exploration of more complex structures, such as enzymes (Bennie et al., 2019). Unlike 2D representation (text or images), the 3D structural information of molecules can be easily accessed by students in iVR (Won et al., 2019). Similar findings in relation to the benefit of intuitive interactivity of iVR have been reported, especially in the field of geoscience (Bagher et al., 2022; Šašinka et al., 2019). In chemistry, understanding 3D molecular arrangements was particularly useful for predicting chemical reactions and properties (Stieff et al., 2005; Wu & Shah, 2004). For example, students' understanding of the 3D hexagonal pattern of ice lattice helped students to explain the formation of snowflakes in this study. Compared to their explanation after magnetic models, students in this study provided a richer explanation of snowflake formation after iVR (see Table 4.8). The findings suggest that by interacting with complex structures in iVR activity, students could close the gap between molecular and macroscopic levels.

However, the complex structures in iVR may be too complex for some non-chemistry undergraduate students in this study. As shown in Table 4.7, students, regardless of their prior knowledge, seemed to regress in terms of representing the concepts of hydrogen bonding after iVR. Poorer learning performances after iVR intervention have been reported by Parong and Mayer (2021). They found that iVR gave extraneous cognitive load and emotional arousal, which hindered learning. Cruising the iVR environment without having control may be the reason for students' negative evaluation. However, unlike Parong and Mayer (2021), this study gave students more control over what they saw. The unexpected results after iVR found this study were perhaps due to the demanding task of relating the microscopic and macroscopic levels of chemistry. Students seemed too focused on highlighting a bigger hexagonal structure, so perhaps they got confused with representing a more detailed hydrogen bonding after iVR. These students were unfamiliar with tasks involving many molecules because chemistry classes typically emphasised the single-molecule perspective (Talanquer, 2011). During the drawing task after iVR, students could be guided to draw hydrogen bonding between two water molecules first before expanding it into a bigger structure.

Interacting With People. Compared to their interaction during the activity with magnetic models, students collaborate more with their peers in iVR (See section 4.8.2). This is perhaps because students were more likely to share the models in iVR environments. As shown in previous studies of computer-supported collaborative learning (Jeong & Hmelo-Silver, 2016), collaboration between students can be fostered by giving the group equal access and control to the task. However, simply having the same task with peers and asking them to collaborate did not always lead to a productive discussion (Dillenbourg, 1999; Webb, 2013). The balance between sharing the same task or visualisation and having enough divergence to trigger discussion has been reported to be effective in supporting collaboration (Liu et al., 2021). To support that, this study found that in iVR, students have the same source of information (the 3D structures) but with enough opportunity to interpret the same source differently. For example, students assumed different positions to see the structures from different angles and noticed different features, which fuelled the discussion (e.g., Nigel-Jasper in section 4.4.5). Other iVR studies have explored the idea of giving students different views of the virtual environment to promote collaboration (e.g., Price et al., 2020; Thompson et al., 2018). But unlike those studies, this study placed both students in the same iVR environment instead of only one student, which could be the reason why many students in this study felt that they were more "in this (space/task) together" with their peers.

6.2.2 Students' Perceptions: Collaborative Exploration or Problem-Solving Activity

Chapter 5 (section 5.2) presented students' perceptions of their experience with iVR in response to Research Question 2(b): "How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation within an *immersive virtual reality* environment?"

Most students in this study expressed enjoyment of being immersed in an environment different from the familiar real space (See section 5.2.1). This finding echoes many iVR studies that increased students' learning motivation by means of transporting students to places that were too far away (Madden et al., 2020), too dangerous (Feng et al., 2020), or too small to reach (Parong & Mayer, 2018).

Having experienced both magnetic models and iVR, students tended to compare both media in their evaluation of iVR (See section 5.2.2). Unlike magnetic models, almost all students highlighted the pedagogical aspects of the activity (narrative and social) in addition to the technological aspect (visual and interactivity). Notably, students' perceptions of technology played a significant role in shaping how the technology impacted their learning, as Gerjets and Hesse (2004) noted. The difference in how students perceived their experience with magnetic models and in iVR implies that students approached the activity with the magnetic model differently than they did with the iVR activity in this study.

While students generally have similar perspectives of magnetic model activities, evaluating students' perceptions of iVR revealed two general views of the experience (See section 5.2.5): iVR as a collaborative space/activity for (1) exploring the presentation of 3D structures and (2) problem-solving. As shown in previous studies on computer-supported learning environments, evaluation of students' perceptions could reveal their different learning approaches to the medium (Klopfer & Squire, 2008).

Exploration Activity. These students appreciate the opportunity to explore 3D structures and notice information in new and engaging ways. Students discussed the ease of visualising 3D molecular structures compared to other media. Unlike with other 3D virtual visualisations, such as desktop VR, students in this study reported that the 3D objects looked like real objects. This showed that iVR addressed the difficulties in controlling or manipulating 3D virtual objects that were often reported in desktop interfaces (Cockburn & McKenzie, 2002). Some students in this study did not even want to walk into the 3D structures inside iVR to avoid ruining the structures. The realistic quality of the object offered by iVR not only increased engagement but also allowed students to easily observe the 3D object from multiple angles, as also shown by Qin et al. (2020). In previous studies, 3D visualisation of molecular structures was commonly displayed on 2D screens, which demanded students' effort to translate the 2D display into 3D (Wu et al., 2001). However, in iVR, the sense of depth was preserved, making it easier for students to gather 3D spatial information (Gerig et al., 2018).

Students seemed to prefer examining the intricacies of complex 3D structures without necessarily participating in the construction process (See section 5.2.2). According to these students, assembling complex 3D structures without enough step-by-step guidance was too challenging. Perhaps these students were used to the common approach adopted by previous 3D chemistry visualisation tools, such as observing 3D visualisation from multiple angles (Sanger & Badger, 2001) or watching animations of 3D molecules (Tasker & Dalton, 2006).

Students appreciated that the tasks were designed from simple towards complex structures, which made them feel that they had just enough support to build their conceptual understanding (See section 5.2.3). Directly going into complex, open-ended tasks overwhelmed students and pushed them to resort to superficial scientific understanding (Hannafin & Land, 2000). A previous study reported that a gradual increase in task complexity only helped students with low prior knowledge, not the ones with high prior knowledge (Großmann & Wilde, 2019). In connection to this study, pairs with alternative prior knowledge slightly outnumbered pairs with higher prior knowledge who appreciated the incremental increase in task complexity. This is perhaps because the tasks in the iVR activity in this study were challenging even for some students with better content knowledge. As observed in students' interactions in iVR, scaffolding was beneficial to encouraging productive interactions with the task. These students also reported that they had more opportunities to consolidate their understanding of iVR. The progression of task complexity has also been used in other educational chemistry studies to give students the opportunity to gradually link their ideas (Broman et al., 2018).

For these students, sharing the exploration of the 3D space with another student was motivating and good for exchanging ideas. Some of the tasks in the iVR activity were difficult for these students, and they felt they could persevere only with the support of their peers. As shown in Waite and Davis (2006), group work not only fostered the generation of new ideas but also enhanced congeniality and motivation to learn. When students work in a socially comfortable environment, they can engage in scientific discussions (Barron, 2003). In relation to avatars, a small number of students in this study did not fully embody the avatar because they did not have facial expressions (See section 5.2.4). Suh (2023) suggested that the ability to customise the avatar with facial expressions helped students embody the avatar and communicate in an iVR environment. Perhaps future studies could include social features to allow students to extend their physical identity in iVR space.

Problem-Solving Activity. These students perceive iVR as an interactive space that challenges them to be active in finding solutions. Again, they compared the challenges of manipulating 3D objects in other media, especially the complex 3D structures. With a "realistic" visual and "easy" interactivity, students felt they were free to try out their ideas about 3D spatial arrangements of water molecules in iVR. Similar to the Predict-Observe-Explain (POE) approach (Treagust et al., 2014), students first predict, experiment, and provide an explanation of their experiment in this iVR activity. This sequence of tasks allowed students to better integrate the chemistry concepts: by predicting, students activated their prior knowledge, and then by experimenting, students observed the consequences of their actions before they finally constructed their ideas into scientific explanations (Chang & Linn, 2013). Students highlighted the importance of getting a different view of the 3D structures to discover new ideas crucial for solving tasks (See section 5.2.2). Students' appreciation of the ease of manipulation in iVR suggests that iVR could facilitate the active learning approach these students have.

Students were pleased to tackle the challenging tasks in iVR, seeing it as a venue to boost their problem-solving skills (See section 5.2.3). The narrative approach in this study was different from previous iVR studies in that it mostly included a single task to observe a particular structure (e.g., anatomy in Zinchenko et al., 2020, or simple molecular structure in Fujiwara et al., 2020) or a predetermined storyline in which students follow a step-by-step procedure (Makransky et al., 2019b). Those approaches adopted by previous iVR studies gave a similar effect to a didactic learning approach that usually resulted in positive learning performance in recalling a list of isolated science concepts. Challenging open-ended tasks gave students more agency in their learning (Cavagnetto et al., 2020). In comparison to more didactic learning approaches, student-driven learning allowed students to choose which concepts were meaningful so that they could link and retain the concepts longer (Taber, 2015). Similar iVR studies showed that students could link several concepts and provide a richer explanation after engaging in ill-defined tasks in iVR (e.g., interpreting test results to diagnose patients in Zackoff et al., 2020). However, not all students appreciated the challenging task in the present study. The findings suggest that when students perceived that the challenging task was appropriate for their ability, they were more likely to engage in the task and gain more scientific ideas. This observation aligns with the flow theory (Nakamura & Csikszentmihalyi, 2014), which states that experience becomes enjoyable when students perceive that the task matches their capacity to perform.

Students perceived that they were collaborating more with their peers in iVR activities compared to the activities with magnetic models in this study (See section 5.2.4). Students saw that collaboration is an integral part of the problem-solving process – without it, they could not complete the challenging task. This iVR activity also afforded students a new way to communicate with their peers. Most students in this study embodied the avatars as if they were their and their peers' real bodies, which allowed them to communicate through non-verbal means, such as gestures (Suh, 2023). The unique capability of iVR in synching physical and virtual bodies afforded embodied communication that can foster collaborative behaviour and task performances. For these students, iVR was a *sociable* media (Kreijns et al., 2022) where they could effectively communicate with their peers. Acknowledging their peers and using gestures were some of the key factors that students mentioned for successfully solving the tasks in iVR.

6.3 Addressing Challenges in Chemistry Learning With Magnetic Models and in iVR

The evaluation of students' interactions, learning outcomes, and perceptions of their experience of learning media in this study seemed to corroborate with each other (See sections 4.8, 5.1.5, and 5.2.5). From those evaluations, the educational benefits of magnetic models and iVR in addressing students' difficulties in learning chemistry are identified and presented below.

6.3.1 Visualising the Abstract Concepts

In chemistry lessons, molecular interactions were typically shown as a 2D representation between two molecules (Bucat & Mocerino, 2009). Without understanding molecular interactions in 3D space, students struggled to explain emerging chemical properties (Tümay, 2016). This study showed that magnetic models and iVR could support students' 3D visualisation of molecular interactions and structures.

Molecular Interactions. Magnetic models benefited students, especially the ones with alternative prior understanding, in learning the O-H attractions between water molecules (See section 4.8). Despite not having the tactile feedback like in magnetic models, students still felt they were "actually touching and manipulating" the molecules and were able to discuss the nature of hydrogen bonding in iVR. According to embodied cognition theory, learners' physical actions contribute to the formation of understanding and representation of the world (Shapiro & Stolz, 2019). Enacting the dynamics of molecular interactions by pushing, pulling, and shaking the reified water molecules gave students a sensorimotor representation to assist in the integration of the concepts with their prior knowledge (Stull et al., 2018). For example, students who enacted the movement of molecules were better at explaining the vaporisation process at molecular levels than students who did not (Langbeheim & Levy, 2018). Magnetic models and iVR provide more information (shape, size, attraction, and repulsion) through haptic and visual cues, which could help students retain the information longer than students who learn through verbal or text (Stull & Hegarty, 2016).

The positive relationship between learning performance and active manipulation can be explained by embodied learning theory (Barsalou, 2008; Shapiro & Stolz, 2018). However, the manipulation of the 3D objects needs to be congruent with the concepts learned. For example, in Makransky et al. (2019b), students have limited interaction with the virtual laboratory apparatus, which may be the reason why students' learning performances between desktop and iVR interventions were comparable. In this study, the actions of pushing and pulling were congruent with the learning goal – molecular interaction (hydrogen bonding). Thus, the effect of embodied actions can be seen in students' performance.

Some ideas about molecular interaction could be better explored in iVR than with magnetic models. Novices tend to forget that models are not true copies of reality (Coll, 2006). With an incomplete understanding of what concepts were being highlighted by particular models, students can develop an alternative understanding (Treagust & Chittleborough, 2001). For example, in this study, the magnetic models were stuck to each other without gaps, prompting the students not to consider the relative length of covalent bonds and hydrogen bonds (See section 4.2.3). Whereas in reality, hydrogen bonds were mostly longer than covalent bonds (Arunan et al., 2011). Seeing no gaps between the magnetic models also made students disregard the difference between inter and intramolecular bonds. This behaviour was evident when students engaged with the models (See section 4.4.3). Unless they actively pull apart O and H atoms between and within the magnetic models, students could not see the difference between covalent and hydrogen bonds. In iVR, hydrogen bonds were explicitly represented, making the ideas of distance and the difference with covalent bonds clearer (See section 4.2.5). The limitations of visualisation tools, such as magnetic models, need to be made explicit so that students can support their learning using the models (Treagust & Chittleborough, 2001). Moreover, this study showed that the interactive use of the models (pulling them apart, rotating, and combining them) was more beneficial than passively viewing them, as reported by Roberts et al. (2005).

Molecular Structures. Providing many models of water molecules during activities with magnetic models and iVR facilitated students' learning of the possible 3D formation when multiple water molecules interacted. However, magnetic models were limited in supporting the explorations of complex 3D structures. Students tend to rely on visualisations of molecules to explain how molecules behave (Coll, 2006; Harrison & Treagust, 2000). Consequently, when attempting to construct a lattice resulted in failure, it impeded students' progress in developing scales and 3D growth.

Constructing complex structures in iVR helped students discover and link several chemistry concepts. This study found that students who successfully constructed and gave positive comments about manipulating complex structures were more likely to engage in richer scientific discussions (See sections 4.6.5 and 4.7.5). This observation aligned with previous studies on embodied actions that showed that students who directly manipulated the 3D objects performed better than those who passively observed the 3D objects (Jang et al., 2017; Johnson-Glenberg et al., 2021). So far, exploration of embodied actions in science learning has been limited because it was difficult to manipulate or enact the movement of abstract concepts (Georgiou & Ioannou, 2019). However, this study showed that these scientific abstract concepts can be reified in iVR to allow more authentic embodied actions, such as constructing progressively bigger structures to enact snowflake growth.

6.3.2 Contextualising Chemistry Ideas

Piece-meal delivery of chemistry concepts was commonly adopted in chemistry classes (Orgill et al., 2019). However, the silos of chemistry ideas made students face difficulties in explaining chemical systems or natural phenomena (Ho, 2019). This study found that incorporating challenging tasks and real-life context (snowflakes) during activity with magnetic models and iVR helped students to link different chemistry ideas to explain the formation of snowflakes.

Using snowflakes as a context during the activity with magnetic models and iVR gave students the opportunity to link basic concepts of molecular structure and interactions. As shown in students' explanations of snowflake formation after iVR, students linked various ideas, such as hydrogen bonding, tetrahedral subunit, and 3D directional growth, in their reasoning (See Table 4.8). This finding supported the movement to include context in students' chemistry learning (King, 2012). In comparison to students' explanations of snowflake formation after magnetic models, students' reasonings after iVR were richer even though the context of snowflakes was included in both learning activities. They have yet to consider other ideas, such as scales, subunits, and 3D growth, in their explanation of snowflakes after magnetic models (See Table 4.8). This finding suggests that students required relevant information to build up their reasoning in contextual learning, and iVR seemed to support the discovery of more relevant information.

The reason for students' ability to link more ideas in iVR could be related to the increased freedom to complete more complex tasks in iVR. This finding supported the notion that students can learn better when the tasks are more complex, such as more open-ended (van Merriënboer et al., 2006) or less passive (Jang et al., 2017; Stillman, 2000). According to the social constructivist perspective, meaningful learning takes place when students actively make connections between the task/environment and their prior knowledge. One of the ways to assist meaningful learning is by giving a complex, challenging task to expose students to the gaps in their prior knowledge so that they can better monitor it and build upon it (Taber, 2010). However, the implementation of challenging tasks in iVR should be done with caution, as not all students appreciate the challenge (See section 5.2.2).

In an iVR environment, student pairs with higher prior knowledge were more likely to successfully construct complex structures and discuss more chemistry ideas. Constructing the complex structures was perceived as challenging by many pairs of students in this study (See section 5.2.2). Although some of the pairs with higher prior knowledge struggled, most of them appreciated the challenges because they could rely on their own ability to solve the problem. In contrast, students with lower prior knowledge were more likely to struggle and wish for more hints. This is supported by previous studies that showed that students with less relevant background knowledge benefitted more in tasks with more guidance or scaffolding (Chernikova et al., 2020). When students can engage in the task without feeling overwhelmed, they can discover new ideas from the task and develop better conceptual understanding (Taber, 2015). Perhaps the tasks were too overwhelming for students with insufficient relevant knowledge to notice past the salient surface features. Scaffolding can assist students in noticing relevant ideas presented in the environment, not just the ones that are salient (Goldman, 2003).

6.3.3 Discussing Chemistry Ideas

Chemistry lectures were still predominantly adopted at the undergraduate level, with assessments to test students' ability to recall information (Bleicher et al., 2003). Therefore, students tend to memorise chemistry terms or use algorithm approaches to answer exam questions correctly (Osborne, 2002). This study showed that interacting with peers during iVR activity could help students engage in meaningful use of chemistry ideas. At the beginning of the session, students mentioned terms such as "hydrogen bonding" to answer questions (See section 4.2.1). But, as they interacted more with the interviewer and their peers, their tendency to simply mention chemical terms seemed to be replaced by a cycle of asking questions and elaborating ideas (See section 4.2.5).

Collaboration could be enhanced by giving students sets of tasks to describe and explain their exploration to their peers (Kirschner & Kreijns, 2005). However, as shown in the findings, having two students together in the activity with magnetic models did not always result in a scientific discussion between peers. Students demonstrated more collaborative interactions in iVR by engaging in a repeated cycle of eliciting ideas and asking questions with peers. This observation was corroborated by students' self-evaluation of their experience with these learning media. The change in social dynamics from activity with magnetic models to iVR activity could be related to the presence of a perceived authoritative source (Hübscher-Younger & Narayanan, 2003) and the access to the representation tool (Jeong & Hmelo-Silver, 2016).

Being immersed inside the iVR space together with peers without external intervention promoted students' collaborative learning. In iVR, the peers provided not only cognitive support through alternative perspectives and feedback but also affective feedback. This does not mean that students can collaborate more without the presence of a teacher. As reported by van Leeuwen and Janssen (2019), teachers can positively affect students' collaboration by giving feedback, prompting and questioning students, and transferring control of the learning process to students. In magnetic model activity, students might be expected to get feedback from the interviewer instead of from each other because the interviewer was asking questions. Students' perceptions of authoritative sources could influence how students socially interact and engage in scientific discussions with peers (Hübscher-Younger & Narayanan, 2003).

This study found that student pairs who shared their task (the 3D objects) with their peers were more likely to engage in collaborative discussions (See section 4.8). During the activity with magnetic models, pairs who shared their models asked more questions with each other – these pairs happened to be dyads with higher prior knowledge. However, during the iVR activity, students tend to share their tasks regardless of their prior knowledge. Previous studies have shown that students who are highly engaged in joint tasks exhibit productive discussion and conceptual changes (Tao & Gunstone, 1999). As noted by Jeong and Hmelo-Silver (2016), technology can support collaboration by providing mutual ground for students to engage in joint tasks. In the iVR activity in this study, students cannot complete the complex task if they divide the task individually. For example, in the construction of a single layer of ice, students have to connect the correct clusters one at a time. This sharing of tasks in iVR improved positive interdependence and individual accountability among students, fostering traits conducive to collaborative learning (Kreijns et al., 2003).

Chapter 7. Conclusions

This study evaluates students' conceptual changes, interactions, and perceptions of their experience with magnetic models and within the immersive virtual reality (iVR) environment. Unique educational benefits of iVR compared to magnetic models are identified from cross-case analysis of students' interactions and interviews concerning their experience with the media. This chapter summarises the major findings of this study along with the significance, implications, recommendations for future studies, and limitations.

7.1 The Summary of Major Findings

Immersive virtual reality (iVR) has become increasingly affordable, which allows more researchers to explore the educational benefits of iVR in recent years. Previous iVR studies commonly used students' self-evaluation of iVR experience and single-tier multiple-choice questions to evaluate the benefits of iVR (Matovu et al., 2022). Although the advantages of iVR to enhance learning engagement have been reported, the potential of iVR to support students' scientific discussion and understanding beyond simple recall has yet to be explored (Hamilton et al., 2020).

In this study, the context is chemistry learning for first-year students. This study employed a multimodal (Jewitt, 2013) and cross-case analysis (Merriam & Tisdell, 2009) to qualitatively analyse students' interactions, conceptual changes, and interviews during the learning activities with magnetic models and iVR. Depending on the student pairs' background knowledge and group composition, each pair exhibited unique learning interactions that resulted in differential learning outcomes. Students perceived the activity with magnetic models as a tactile, hands-on individual activity to learn the nature of hydrogen bonding. In contrast, students perceived iVR activity as a collaborative space to explore the intricate 3D molecular structures or develop problem-solving skills to explain snowflake formation.

7.1.1 Students' Interactions and Changes in Conceptual Understanding of Hydrogen Bonding and Snowflake Formation

These research questions addressed students' interaction with magnetic models and within the iVR environment to achieve conceptual changes. The chemistry ideas being investigated are hydrogen bonding and snowflake formation.

Research Question 1(a) - How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions when using *magnetic models*? (See sections 4.2.2 – 4.7.2)

Students started the activity with various levels of understanding of the concepts of hydrogen bonding. After the magnetic model activity, students developed a better understanding of O-H attraction between two water molecules. They also developed an understanding of simple molecular structures that can be formed by water molecules, including tetrahedral and hexagonal structures. However, students have not yet considered the length of hydrogen bonds relative to the length of covalent bonds after the activity with magnetic models.

For the concepts of snowflake formation, students noticed the unique symmetrical shape of snowflakes prior to the activity with magnetic models, but they were unsure how exactly water molecules interact to result in such distinct shapes of snowflakes. After the magnetic model activity, students directly match the observed structures to explain the branches or the hexagonal shape of snowflakes. However, students only explained the horizontal expansion of the structure that results in *flat* snowflakes.

The influence of students' prior knowledge and group composition is evident in their conceptual and social interactions during the activity with magnetic models. During their conceptual exploration, student pairs with varying levels of understanding of hydrogen bonding interacted with magnetic models differently. Student pairs with an alternative understanding of hydrogen bonding used the models to revise their idea of O-H attractions between different water molecules, while student pairs with higher prior knowledge explored various molecular structures and their stability. However, magnetic models were limited in supporting pairs of students with higher prior knowledge in their exploration of 3D ice lattices. Prior knowledge influences in social interactions can be seen in how pairs of students with limited prior knowledge focused on their own set of models and interacted more with the interviewer. In contrast, pairs of students with higher prior knowledge were more readily able to share their models, allowing them to talk more to each other and discuss more topics, including hexagonal patterns of snowflakes.

Research Question 1(b) - How do pairs of first-year students change their understanding of hydrogen bonding and snowflake formation through their interactions within an *immersive virtual reality* environment? (See sections 4.2.5 – 4.7.5)

For the concepts of hydrogen bonding, before the iVR activity, students gave some explanation about the optimum angle and distance between two water molecules. After the iVR activity, students explained hydrogen bonds between multiple water molecules in the context of 3D molecular structures. However, some pairs of students did not clearly represent hydrogen bonding between water molecules in their diagrams after iVR.

For the concepts of snowflake formation, before the iVR activity, students did not change their previous explanation of snowflakes or became unsure after realising that water molecules should have interacted in 3D space. After the iVR activity, students highlighted the hexagonal-hexagonal parallel between the 3D ice lattice and snowflakes. Some students also included multiple ideas, such as tetrahedral subunits, growth, and the influence of environmental factors towards the various patterns of snowflakes' branches.

Students' learning experience in iVR encompassed conceptual, spatial, and social interactions. Concerning conceptual exploration, students' conceptual discussion and engagement varied based on their initial prior knowledge and group compositions. Pairs with an alternative understanding of hydrogen bonding mainly focused on the 3D orientation of O-H attraction during the simple structure tasks but did not extend their scientific discussion beyond salient surface features in complex structures. Conversely, student pairs with higher prior knowledge challenged their preconceptions during the complex structure tasks and noticed different 3D features to explain the shape of snowflakes. In relation to spatial exploration, pairs of students performed hands-on and full-body manipulation of 3D structures that were not feasible to perform with magnetic models. Student pairs with extensive explorations noticed more ideas regarding the 3D spatial arrangement of water molecules. A closer look at pairs of students' social exploration revealed task-dependent changes in students' interaction in iVR. Students engaged in more extensive discussion and independent problem-solving during complex structure tasks. However, a tendency to rely on external hints was observed when the hints were available for students.

7.1.2 Students' Perceptions of Their Experience With Magnetic Models and Within iVR Space

These research questions addressed students' perceptions of their learning experience with magnetic models and within iVR.

Research Question 2(a) - How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation when using *magnetic models*? (See section 5.1).

In general, students perceived the activity with magnetic models as a fun individual activity to explore the attraction and repulsion between water molecules. Adopting Dede's immersion features framework (2017), four key features were identified from students' comments in relation to their learning experience with magnetic models. Students mostly highlighted the interactivity (actional) followed by visualisation (sensory) features of magnetic models. Less than half of the students discussed the narrative and social features in their evaluation of magnetic models.

For the sensory feature, students appreciated being able to observe the 3D structures of water molecules. They especially appreciated the benefit of magnetic models in terms of visualising simple structures that comprise multiple water molecules, including tetrahedral and hexagonal structures. A handful of students appreciated the visualisation of a single/two water molecule but also recognised its limitations in showing the difference between hydrogen and covalent bonds.

For the actional feature, students appreciated being able to feel the magnetic pull in relation to their exploration of hydrogen bonding and simple structures. Students highlighted that feeling the attraction and repulsion helped to clarify their understanding of hydrogen bonding (O-H attraction). They talked about the magnet "guiding" them to construct tetrahedral and cyclic structures. A small number of students recognised the limitation of magnetic models in constructing complex structures, such as ice lattices.

For the narrative feature, students appreciated being able to interrogate their prior knowledge of hydrogen bonding and test it using magnetic models. They perceived that the drawing task prior to the magnetic model activity helped them to realise their level of understanding. Very few pairs mentioned the magnetic model activity as a problem-solving task.

For the social feature, students perceived the activity with magnetic models as an individual activity even though they were aware of the presence of their peers. Students explained that the activity did not feel like a collaborative task because they were exploring their own set of models. Less than half of the students appreciated having a partner to share ideas during the activity with magnetic models.

Research Question 2(b) - How do pairs of first-year students evaluate their experience of learning about hydrogen bonding and snowflake formation within an *immersive virtual reality* environment? (See section 5.2).

In general, students perceived the iVR activity as an engaging, collaborative exploration of 3D visualisation or as a collaborative problem-solving activity to apply and consolidate their understanding of hydrogen bonding in the context of snowflakes. Similar to magnetic models, Dede's immersion features framework (2017) was also adopted in the identification of four main features from students' evaluation of their iVR learning experience. All students highlighted the visualisation (sensory) and interactivity (actional) features of iVR. Unlike with magnetic models, almost all students appreciated the narrative and social features when talking about their experience in the iVR environment.

For the sensory feature, students expressed excitement about visualising simple and complex 3D structures. In iVR, students elaborated on how they were able to observe the intricacies of the 3D spatial arrangement of water molecules – something that they could not do easily in their everyday experience and with other media. Students appreciated being able to observe simple structures and, especially, massive complex structures from different angles. In comparison to magnetic models, students mentioned how they finally recognised the 3D expansion of hexagons. A couple of students perceived that the structures looked realistic, so they felt they would ruin the structures by walking through them.

For the actional feature, students highlighted the intuitive interactivity in the iVR environment to easily manipulate 3D molecular structures. They tended to compare their experience manipulating 3D molecules with other media. Unlike other media, students mentioned how it was easy and enjoyable to lift, rotate, or walk around the molecules as if they were interacting with real 3D objects. Students appreciated being able to construct both simple and, especially, complex structures. They explained how it was difficult to construct complex structures with magnetic models.

Two main perspectives about constructing complex structures were identified from students' evaluations. First, half of the students appreciated constructing the complex structures in iVR and felt that the activity contributed to their problem-solving skills. These students were generally successful in constructing the single layer and ice lattice. Second, the other half of the students felt that building the complex structure in iVR was too challenging for them, and they wished they had more hints to complete the task. These students generally had limited prior knowledge or had a more individualistic approach within an iVR environment.

For the narrative feature, students appreciated how the design of the tasks in the iVR activity helped them to learn chemistry better. The elements that students mentioned were the problem-solving task and the stepwise task. For the problem-solving task, students relate to the increased interactivity and agency in iVR, compared to the activity with magnetic models. They felt satisfied to be able to use their own analytical skills to complete the task without external help. The stepwise task was helpful for students because they felt that they had enough opportunities to gradually build their knowledge from basic to more advanced concepts.

For the social feature, students expressed enjoyment in having a partner inside iVR to bounce ideas and feel more motivated to complete the activity. Only one pair wished that they could complete the activity alone. Students also highlighted new ways of communicating due to the avatars. Most students did not feel the lack of facial expressions hindered their social interaction inside the avatar because they could still communicate through voices and gestures. Only a handful of students felt social isolation due to the expressionless avatars.

7.2 Significance

This study addressed the research gaps identified in the literature review in terms of evaluating students' conceptual changes, interactions, and perceptions of their learning experience within the collaborative iVR space. These evaluations were compared to the evaluations of magnetic models to identify the unique educational benefits of iVR. In this study, it became clear that students' backgrounds and group compositions played a significant role in shaping their interactions with learning media and, consequently, impacting their learning outcomes.

Many studies have reported positive learning outcomes after iVR activity (Wu et al., 2020). However, from previous iVR studies, it is still unclear how iVR helped students achieve the observed conceptual changes (Matovu et al., 2022). Moreover, students' conceptual changes were commonly reported as an improvement in memorisation (Hamilton et al., 2020). The in-depth investigation of student pairs' interaction in this study helped to better understand how students utilise iVR to achieve an understanding of hydrogen bonding and snowflake formation. This study found that students' individualistic exploration of attraction and repulsion with magnetic models helped them to understand hydrogen bonding. However, magnetic models cannot fully support their exploration of the 3D lattice, which resulted in a limited understanding of the microscopic/macroscopic scale gap and 3D growth. In contrast, students established a richer explanation of snowflake formation by discussing and collaboratively interacting with more complex 3D structures in an iVR environment. This study also identified how pairs' prior knowledge and group composition impacted their interactions and the extent of their learning and engagement in each activity.

Previous studies have shown that students exhibited positive attitudes toward their learning experience in iVR (Radianti et al., 2020). Yet, students' views were commonly evaluated for their perspective on the technological aspect of iVR (e.g., interactivity, usability). Adopting Dede's (2017) immersion features framework, this study identified not only the technological but also the pedagogical features of magnetic models and iVR from students' interviews after experiencing magnetic models and iVR. Students, in general, hold the same views of magnetic model activity as a fun and tactile individual activity to explore intermolecular interactions. In contrast, students perceived the iVR environment as a collaborative space to (1) explore the presentation of 3D structures or (2) engage in problem-solving tasks. Compared to magnetic models, students were more appreciative of the complex 3D spatial arrangements of molecular structures after iVR activity.

7.3 Implications and Recommendations for Future Studies

This study has practical and theoretical implications for the field of educational technology. Personally, as a person who used to work in an educational technology company developing iVR activities, this study has shown the importance of (1) considering alternative ways to evaluate the benefits of iVR, (2) considering students' experience, and (3) considering the unique benefits of each medium.

The ways to evaluate the learning outcomes of iVR can affect the interpretations of its benefits. Heavy reliance on single-tier multiple choice or self-evaluation Likert scale could limit the evaluation of the extent of students' understanding and perceptions. This study offered alternative methods to evaluate the benefits of education technology: multimodal cross-case analysis of students' interaction, conceptual changes, and perceptions of their experiences with iVR. Although it can be more time-consuming, future studies may wish to consider in-depth qualitative analysis of students' learning journey with the learning medium to unravel its unique benefit.

The educational benefits identified by educators or instructional designers may be realised differently by students. It was evident in this study that students' backgrounds and group compositions contributed to students' interactions with learning media and, eventually, to their learning outcomes. In the context of collaborative learning, future researchers and educators may wish to consider students' prior knowledge and social arrangements when choosing learning media and designing learning tasks.

Each learning medium has its own unique educational benefits. As shown in this study, iVR can support students' scientific understanding of abstract concepts in different ways than magnetic models can. Rather than transferring or using the same design consideration across various learning media, future studies may explore different learning approaches that best suit the key features of each learning medium. Considering the rapid change in educational technology, Dede's (2017) immersion features could be extended or modified for further investigation of the educational benefits of different learning media.

7.4 Limitations

All students experienced learning activities with magnetic models and iVR. The length of each activity was not the same, and the order in which they went through the learning activity first was always the same. Their experience with magnetic models may influence their experience in the iVR learning activity. This limits the discussion of direct comparison of the learning media. Instead of direct comparison to claim which learning medium is the best, this study considered what worked in each learning medium and why it worked. The current setup also seemed fair to students because everyone in the cohort has the chance to experience all learning media. Future studies may want to have different groups of students, each experiencing only one type of learning media.

Students went through all interviews and learning activities as pairs. While this setup worked on recording students' evaluations and learning as a group, it was challenging to assess individual learning. Although most students feel they benefitted from collaborating with their partners, a couple of students prefer to do the experience alone. Future studies may want to compare individual and group learning.

The learning outcomes reported in this study were the product of the one-time interaction of students with the learning media. To better understand the transfer of learning from iVR to their everyday life, including classroom, longitudinal studies involving class observations may be conducted in the future. Future studies may wish to explore different learning topics that can benefit from iVR technology, like biochemistry, geology, or engineering.

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Appendix A: Snowflakes iVR Learning Activity

Students were given explanations of interacting in an iVR environment before they don iVR headsets. The verbal guidance provided by the researcher is as follows:

Discuss and explore in iVR: "*You both are going to share the same iVR space and will be able to see each other. Please think out loud and discuss your thoughts with your partner. Also, make sure you walk around to get a different perspective of the object you will encounter inside the iVR space.*"

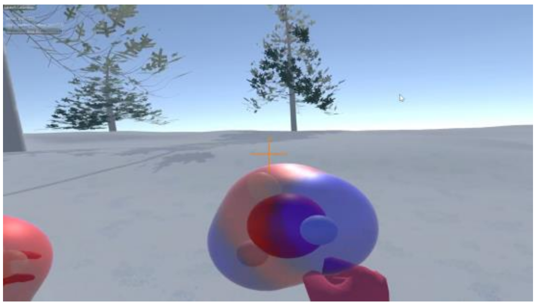
Controllers: "*Use the controllers to interact with the 3D objects inside iVR space. To grab molecules, pull the trigger buttons. To press the buttons inside iVR, simply push them with your hands.*"

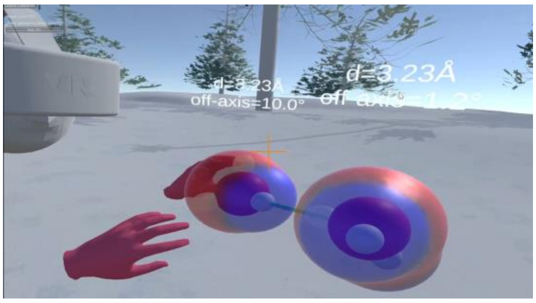
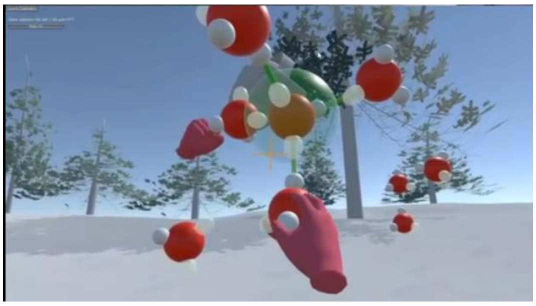
Safety: "*You will see a blue grid when you are getting close to the boundary of the iVR space. When you feel uncomfortable, please let us (the researchers) know anytime.*"

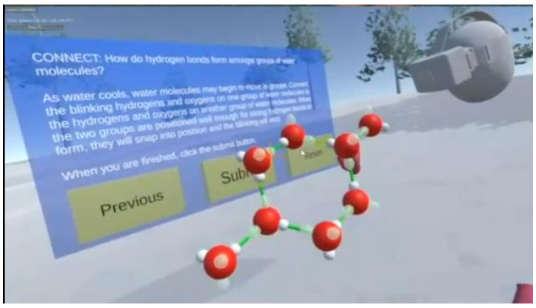
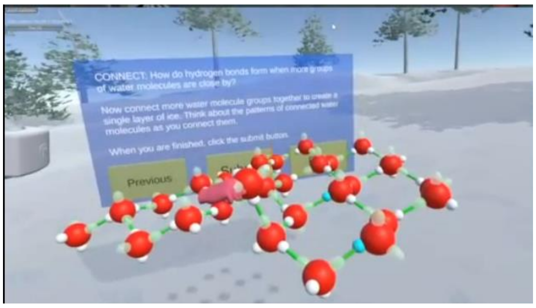
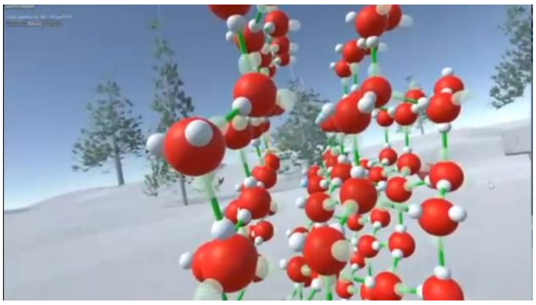
The students then wore the headsets and received audio and text prompts from the iVR program. The following are the instructions for each task in the Snowflakes iVR learning activity.

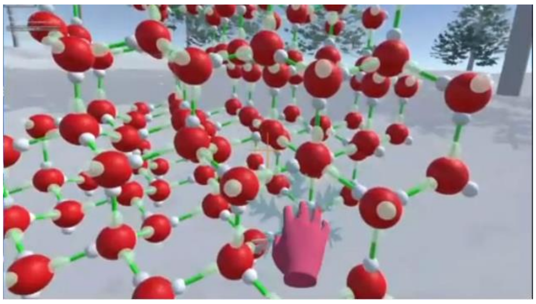
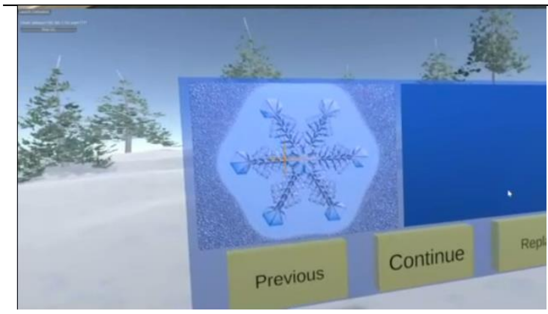
Table A.1

Instructions Inside the Snowflakes iVR Program

Screenshot of learning tasks	Instructions
Winter forest 	Welcome to Winter Wonderland. Have a look around you. What do you notice about the shape of the snowflakes? Discuss why you think these shapes occur, then click the submit button.
Two water molecules (Intro) 	How do you explain the shapes of the snowflakes? To answer this question, we are going to explore the intermolecular forces between water molecules. Let's start with two water molecules. Please click the continue button to begin.

Two water molecules 	DESCRIBE: What are the features of water molecules? Look at the water molecules in front of you. Describe what you notice and what each feature represents. When you are happy with your answer, click the submit button. CONNECT: How do you make a hydrogen bond? Make a hydrogen bond (a green stick) between two water molecules and describe what you notice about the colour and thickness of the hydrogen bond. When you are happy with your answer, click the submit button. EXPERIMENT: How can you make this bond stronger? Adjust the position of the water molecules to make a stronger bond. Discuss the strength of the hydrogen bond in relation to the angle and distance between the water molecules. When you are happy with your answer, click the submit button.
Tetrahedral 	PREDICT: How many hydrogen bonds can form around one water molecule? Now, let's think about hydrogen bonds when more water molecules are nearby. Predict the maximum number of hydrogen bonds one water molecule can form and explain your reasoning. When you are happy with your answer, click the submit button. CONNECT: How many hydrogen bonds can form around one water molecule? Connect as many water molecules as possible to the central water molecule. How does this compare to your prediction? When you are happy with your answer, click the submit button. DISCUSS: How many hydrogen bonds can form around one water molecule? Discuss why the water molecules have four hydrogen bonds and what shape the water molecules form. When you are happy with your answer, click the submit button.

Two clusters of water molecules 	CONNECT: How do hydrogen bonds form amongst groups of water molecules? As water cools, water molecules may begin to move in groups. Connect the blinking hydrogen bonds on one group of water molecules to the hydrogen and oxygens on another group of water molecules. When the two groups are positioned well enough for strong hydrogen bonds to form, they will snap into position, and the blinking will stop. When you are finished, click the submit button. PATTERNS: What shape do the connected water molecules form? Discuss what you notice about the shape of the connected water molecules. Looking just at the hydrogen now, can you see a pattern? How about the lone pairs of electrons on the oxygens? How could you use this information to connect more water molecules? When you are happy with your answer, click the submit button.
A single layer of ice 	CONNECT: How do hydrogen bonds form when more groups of water molecules are close by? Now, connect more water molecule groups together to create a single layer of ice. Think about the pattern of connected water molecules as you connect them. When you are finished, click the submit button. DESCRIBE: What shapes do water molecules form in ice? Describe what you notice about the structure. Make sure you pick up the layer of ice and look at it from multiple angles. When you are happy with your description, click the submit button.
Three layers of ice 	CONNECT: What shapes do water molecules form in ice? Let's make a bigger structure of ice. Connect the bottom two layers first and then the top layer. Make sure you walk around and observe the structure from multiple angles. When you are finished, please click the submit button.

	OBSERVE: What shapes do water molecules form in ice? Pick up the ice lattice and look at it from multiple angles. What do you notice about the shape this time? When you are happy with your description, click the submit button.
Ice lattice and snowflakes 	COMPARE: How can the shape of snowflakes be explained? Now, compare the ice structure you created with the shape of the snowflakes. Discuss what features of the snowflakes you can explain with the ice structure. When you are happy with your answer, click the submit button. COMPARE: What features of snowflakes cannot be explained by the ice structure? This ice lattice contains 150 water molecules. The average snowflake, on the other hand, has approximately 10^{19} water molecules. Compare the numbers and discuss their implications for explaining the shape of snowflakes. When you are happy with your answer, click the submit button.
	Video Explain the environmental factors that influence the formation of snowflakes.

Appendix B: Coding Schemes for Students' Conceptual Explanation of Snowflakes

Table B.1

Coding Schemes for Students' Explanations of Snowflakes

Category	Subcategory	Description
Not sure		Student makes no attempt to explain the shape of snowflakes.
Incoherent or hard to categorise		Students' explanation contains contradicting ideas.
Focus only on the appearance	Flat structures (i.e., branches)	Student focuses on explaining the flat appearance of snowflakes, including the branches of snowflakes.
	Variations in patterns	Student focuses on environmental factors of randomness in molecular interactions to explain why there are different patterns of snowflakes but does not explain the hexagonal symmetry.
Explain molecular interactions in 3D	In terms of hydrogen bonds	Student recognises that molecules in snowflakes interact in 3D but does not explain other features of snowflakes' shapes.
	+ 3D lattices and the variations in patterns	Student recognises that molecules in snowflakes interact in 3D and attempts to explain the different variations in snowflakes' patterns.
Explain hexagonal symmetry	In terms of hydrogen bonds	Student's explanation focuses on the hexagonal symmetry in snowflakes only, but there is no mention of tetrahedral units as the building blocks of the structure.
	+ variation in patterns	Student explains the hexagonal symmetry and variations in snowflake patterns, but there is no mention of tetrahedral units as the building blocks of the structure.
Recognise tetrahedral unit as the building block of snowflakes	In terms of hydrogen bonds or 3D lattice	Student recognises that molecules in snowflakes interact in 3D to form tetrahedral units but does not explain the hexagonal symmetry or variations in patterns.
	+ the hexagonal symmetry	Student recognises that molecules in snowflakes interact in 3D and form tetrahedral units, which result in hexagonal patterns amongst water molecules to explain the hexagonal symmetry in snowflakes.
	+ variation	Student recognises that molecules in snowflakes interact in 3D to form tetrahedral units and explain variations of patterns in snowflakes.
	+ the hexagonal symmetry and the variation in patterns	Student recognises that molecules in snowflakes interact in 3D and form tetrahedral units, explains the hexagonal symmetry, as well as variations of patterns in snowflakes.

Note. Adopted from Matovu et al. (2023b)

Appendix C: Coding Schemes for Students' Evaluation of Magnetic Models and iVR

Table C.1

Coding Schemes for Students' Evaluation of Visualisation and Interactivity with Magnetic Models

		Visualisation	
		1-2 molecules	> 5 molecules
Interaction	Observe	Students used magnetic models to observe features of water molecules (e.g., the size of atoms).	Students used magnetic models to observe features of molecular formation involving more than five molecules.
	Build (appreciate)	Students used magnetic models to feel the attraction and repulsion between two water molecules.	Students used magnetic models to test hypotheses about possible molecular structures (e.g., rings, tetrahedral).
	Build (struggle)	-*	Students have issues using magnetic models to explore molecular structures with >5 molecules (e.g., stability of structures).

Note. (*) This category is not defined because no pairs of students discuss it.

Table C.2

Coding Schemes for Students' Evaluation of Visualisation and Interactivity in iVR Space

		Visualisations		
		Environment	Simple structure (two water mol., tetrahedral)	Complex structure (single-layer, ice lattice)
Interaction	Observe	Students viewed iVR as a means to be transported to various places and observe their surroundings.	Students used iVR to observe simple structures.	Students used iVR to observe complex structures. May not feel confident to "touch" the complex structures.
	Play	-*	Students used iVR to manipulate simple structures and observe them from different angles.	Students used iVR to manipulate complex structures to observe them from different angles.
	Build (appreciate)	-*	Students used iVR to construct simple structures.	Students used iVR to construct complex structures.
	Build (struggled)	-*	-*	Students have difficulty in making complex structures (wished for more hints).

Note. (*) This category is not defined because no pairs of students discuss it.

Table C.3

Coding Schemes for Students' Perceptions of Narrative During the Activities with Magnetic Models and Within iVR Space

Category	Subcategory	Description
Task design	Test hypothesis	Students feel that they have the opportunity to apply their prior knowledge in different contexts to test hypotheses.
	Stepwise task	Students feel that the incremental scaffold (from simple to complex tasks) helps build their understanding.
	Problem-solving	Students feel that they have the agency to figure out the solution to a task. May express appreciation for the opportunity to improve analytical or problem-solving skills.

Table C.4

Coding Schemes for Students' Perceptions of Collaborative Tasks During the Activities with Magnetic Models and Within iVR Space

Category	Subcategory	Description
Group play	Bounce ideas	Students appreciate having a partner because it helps them to bounce ideas/ construct knowledge.
	Fun	Students appreciate having a partner because it motivates them to complete the task or makes the experience fun. May talk about how being with a friend encourages them to interact and complete the task.
	Faster	Students appreciate having a partner because it helps them to complete the task faster.
	Less awkward	Students appreciate having a partner because it helps them to feel comfortable performing the task. May express awareness of people (researchers) watching.
Individual play		Students prefer to experience iVR alone.

Table C.5

Coding Schemes for Students' Perceptions of Communication Modes Within iVR Space

Category	Subcategory	Description
Avatars (no facial expression)	Adapted	Students used voice, gesture, or both to maintain social connection/ communicate inside the iVR space.
	Struggled	Students wished they could see each other's faces or full-body avatars. May express the loss of social interactions due to the lack of facial expression.
	Confident	Students feel more confident talking in iVR. The reason may include being anonymous inside iVR (generic avatar).
Hybrid space	People	Students were conscious of people outside iVR that are not represented by any avatar inside iVR.
	Spatial	Students were conscious of the environment outside iVR that cannot be seen inside iVR (e.g., wall).

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Students' Use of Magnetic Models to Learn Hydrogen Bonding and the Formation of Snowflakes

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