Augmented Reality Training System Fusing the Triple Nature of Chemical Concepts

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Abstract

Understanding chemical concepts requires learners to engage with information on three interconnected levels: the macroscopic (observable phenomena), the microscopic (atomic and molecular interactions), and the symbolic (chemical equations and representations). This triple nature of chemistry poses challenges for traditional teaching methods, particularly when conveying the abstract and invisible aspects of these concepts. As a result, gaps in comprehension can arise, ultimately hindering learning outcomes. This paper presents the design and implementation of an Augmented Reality (AR) training system fusing the triple nature of chemical concepts into a contextually coherent learning experience. By integrating AR technology, learners can interact with 3D models of molecules, visualise chemical reactions in real-time, and connect abstract symbols with their physical and molecular counterparts.

Keywords

chemistry learning, augmented reality, interactive systems, learning and education, head-mounted displays

1. Introduction

Experiential learning or learning by doing is a well-established educational approach that enhances students' comprehension of concepts taught in the classroom [1, 2]. For example, in chemistry education, laboratory activities play a vital role, allowing students to manipulate substances and handle laboratory equipment to conduct and observe chemical reactions, and understand new chemical concepts. Learning chemistry and understanding chemical concepts requires engagement on three interconnected levels, collectively known as the triple nature of chemical concepts. These levels include:

- Macroscopic: this level focuses on observable phenomena such as reactions, properties, and behaviours of substances in bulk. It includes concepts like concentration, temperature, and pressure, emphasising measurable quantities and tangible observations.

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- Microscopic: this level examines the behaviour and interactions of individual atoms and molecules. It involves understanding structures, bonding, and the forces that govern molecular interactions, providing insight in how macroscopic properties arise from microscopic behaviour.
- Symbolic: this level uses chemical symbols, formulas, and equations to represent the other two levels. It encompasses the language of chemistry, including chemical equations to describe reactions, the periodic table, and other notational systems that help convey complex ideas in a concise manner [3].

Traditional teaching methods often face challenges in effectively conveying the abstract and invisible nature of chemical concepts, which ca result in gaps in comprehension. To address this, educators frequently incorporate various training systems, particularly at the microscopic level, enabling students to develop a deeper understanding of specific chemical concepts [4, 5]. Visualisation tools for the microscopic level include static and dynamic 2D or 3D micro-representations, such as 2D static images, 3D physical static models, 2D or 3D animations, as well as virtual reality models [6, 7]. Notably, research indicates that students who engage with 3D animations tend to achieve a better grasp of the chemical concepts compared to students using static representations [8].

Augmented reality (AR) enhances the physical environment by overlaying it with computer-generated elements. This enables students to develop important skills and literacies that are difficult or impossible to achieve in traditional technology-enhanced learning environments [9, 10]. In this paper, we present the design and implementation of an AR training system designed to fuse the triple nature of chemical concepts. By integrating AR technology, learners can interact with 3D models of molecules, observe chemical reactions in real-time, and connect abstract symbols with their physical and molecular counterparts.

2. Design AR Training System

As mentioned, understanding chemical concepts requires learners to engage with information across three levels. However, in traditional classroom settings or laboratory, presenting all three levels simultaneously within the same context can be challenging. Additionally, it is often difficult to ensure that information at one level is effectively connected to the others. Achieving a seamless coupling of these levels is likely to result in coherent understanding of a complex chemical concept and improve learning outcomes. The primary objective of designing our training system is to facilitate this seamless coupling of information across the three levels.

This coupling can be achieved through AR due to its ability to overlay visual content onto the physical world. By making invisible elements visible to the naked eye, AR allows us to seamlessly integrate all three levels within the real world context, such as a laboratory experiments. The design of our training system is presented in the following sections.

2.1. Combining Macroscopic, Microscopic and Symbolic Levels of Information

When designing an AR system, the goal is to create experiences that integrate seamlessly with the surrounding environment, enhancing rather than obstructing or replacing reality. To

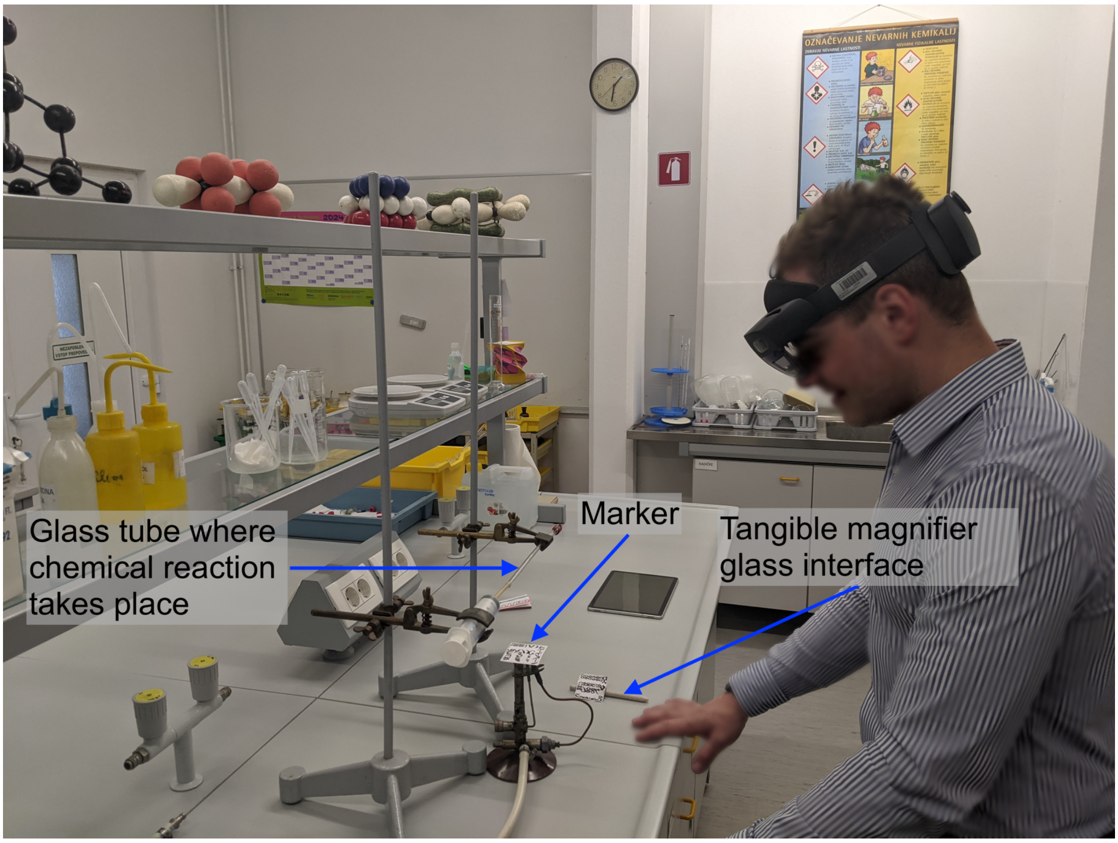

Figure 1: Laboratory setup in which the training is deployed. The observable phenomena occurs within the glass tube. The figure also shows a MARKER, which is used for positioning the visualisation and the TANGIBLE MAGNIFYING GLASS INTERFACE used to manipulate the VIRTUAL MAGNIFYING GLASS.

improve the understanding of chemical concepts, we use the laboratory settings (Figure 1) as the physical context, where experiments represent the macroscopic level of information (i.e. the observable phenomena). Since learners need to interact with laboratory equipment, it is essential for the tool being designed to enable hands-free interaction; otherwise, it would hinder their ability to conduct the experiments effectively. Therefore, we opted for a head-mounted optical see through display (Figure 1).

To visualise the microscopic level of information (i.e. atomic and molecular interactions), it is essential to establish a method for transitioning from macroscopic level to the microscopic level. For this purpose, we designed the VIRTUAL MAGNIFYING GLASS, which allows the user to explore the microscopic level of information while preserving the context of the experimental setup (Figure 2 left).

The final level of information to be visualised in the laboratory experiment is the symbolic layer. To incorporate this, we place labels above each interacting particle indicating the symbolic description of the molecule. Additionally, we have carefully designed molecule models to align with these symbolic descriptions. This is achieved though consistent use of colour, which indicates the type of atoms (e.g. blue for Nitrogen), the number of atoms (e.g. consistent with

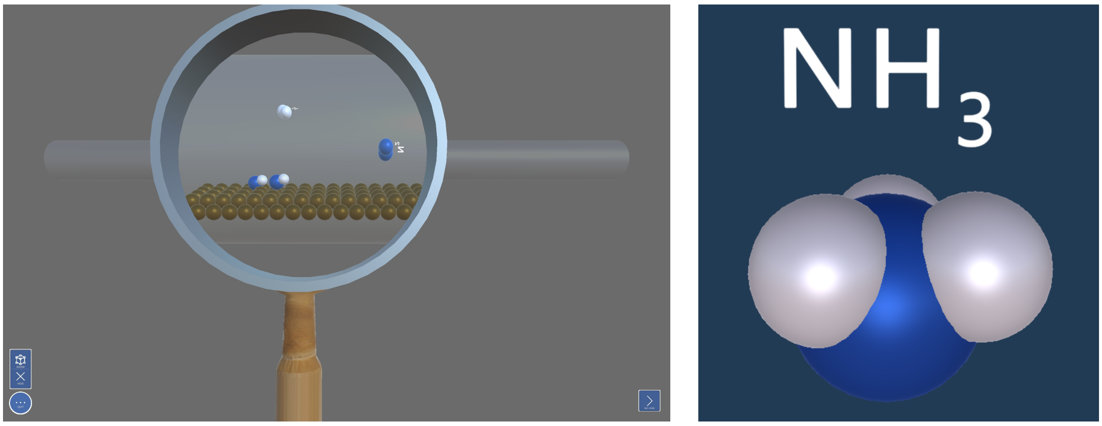

Figure 2: Left—The virtual magnifying glass simulates the transition from macroscopic to microscopic level of information. Atomic particles become visible only when viewed through the magnifier. Right—A 3D model of an ammonia molecule with symbolic notation NH_3. Nitrogen atoms are modelled as blue spheres, while hydrogen atoms are modelled as white spheres, with their sizes scaled proportionally to their actual dimensions.

symbolic description) and the relative size of atoms (e.g. Nitrogen atoms are represented by larger spheres compared to hydrogen atoms) (Figure 2 right).

2.2. Interacting With Virtual Magnifying Glass

One method to designing interaction with the virtual magnifying glass could be fixing it in space and prompt learners to peak through it by moving to the predefined position where educator has placed the glass. To make the tool more engaging we decided to allow learners to handle the virtual magnifying glass. When designing this interaction we tapped into existing affordances of handling a real magnifying glass where the interaction consists of grasping the handle and moving it in order to look at the point of interest. We implemented this interaction following two approaches: (i) through tangible object held in hand that acts as a proxy to manipulate the virtual magnifying glass position and (ii) through a mid-air grasping gesture combined with hand movement.

3. System Implementation

We implemented two prototype systems for visualising chemical concepts, one using an AR head-mounted-display (HMD) Microsoft HoloLens 2 and the other on a 10.5, ∈ Android tablet Samsung Galaxy Tab S4. The two prototypes were developed to evaluate their effects on learning outcomes when learners (future chemistry teachers) study the same content on a traditional display compared to in-context AR display. The development has been done iteratively with the experts in chemistry didactics. Their constructive feedback after each system iteration has assured the correctness of all visuals as well as improved the user-friendliness of interaction.

3.1. Implementation of the AR prototype

The AR prototype was implemented for Microsoft HoloLens 2[1] using the Unity3D game development engine[2]. For camera pose tracking, the HoloLens inbuilt tracking system was used. To initialise the positions of augmentations, we used Vuforia[3] and our custom-made image markers, which accurately align the virtual content with physical chemistry experiment setups. One marker is used for initialising the experiment setup of the chemical concept and is removed from the scene after initialisation. Another marker is used for tracking the physical tangible object, which acts as a prop to manipulate the virtual magnifying glass position. The marker is continuously tracked throughout the learning scenario.

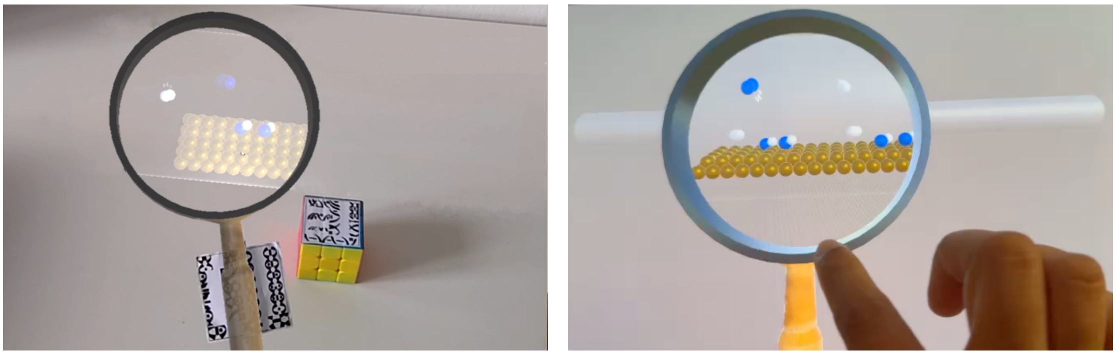

Figure 3: Left—Interacting with the AR version of the system through the prop in hand: NH_3 formation learning scenario. Right—Interacting with the tablet version of the system through touch interactions: NH_3 formation learning scenario.

All molecular 3D models, including both interacting and non-interacting molecules, as well as relevant confounding factors, were developed as prefabs in Unity 3D. This modular design facilitates easy instantiation, manipulation, and scalability of the models within the simulation. A spawning mechanism was developed to generate non-interacting molecules dynamically. These molecules were designed to spawn at specified locations and move freely, which enhanced the realism of the simulation. To enhance user control, a button was integrated into the interface, allowing learners to toggle the visibility of non-interacting molecules. This feature enables learners to customise their view, focusing on specific interactions or phenomena without distraction.

Learners can observe chemical reactions through a virtual magnifying glass, a key feature of the experience. The virtual magnifying glass was designed as a 3D virtual object within the AR space and can be manipulated in two primary ways:

1. Using a tangible object in hand which acts as a prop: A tangible object was attached to the marker (Figure 2 right), allowing learners to directly control the virtual magnifying glass. As learners move the object, a corresponding virtual magnifying glass

[1]https://www.microsoft.com/en-us/hololens
[2]https://unity.com/
[3]https://developer.vuforia.com/

appears above the marker with continuous tracking, allowing the observation of chemical interactions in detail.

2. Grasping the virtual object which is fixed in space: Using the HoloLens's hand tracking and mid-air gestures, learners can also grab and reposition the VIRTUAL MAGNIFYING GLASS with their hands.

To control the visual effects, a new shader was implemented for the lens of the VIRTUAL MAGNIFYING GLASS. This shader creates a magnifying effect that enhances the visibility of molecules and chemical interactions, rendering them only through the lens.

3.2. Implementation of the Tablet Prototype

The tablet version of the prototype was also implemented using the Unity 3D development environment, but deployed on a Samsung Galaxy Tab S4 [4] tablet. Its functionality is similar to the AR prototype, ensuring consistency across platforms.

The tablet interface was designed with touch interactions. In this implementation, learners can tap and drag the VIRTUAL MAGNIFYING GLASS on the touchscreen to explore chemical reactions in detail. The visual design of the tablet application mirrored that of the AR version, featuring similar colour schemes, layout, and interactive elements.

4. Conclusion and Future Work

This paper presents an AR training system designed to enhance the understanding of chemical concepts by connecting the macroscopic, microscopic, and symbolic levels of chemistry. By using AR technology, learners can engage with 3D models of molecules and visualise chemical reactions in real-time, making abstract ideas more accessible.

The initial feedback from the experts in chemistry didactics has been positive. They recognise the value of combining immersive visuals with user-friendly controls to overcome the limitations of traditional chemistry education, and aim to explore its effectiveness through comprehensive user evaluation. We are currently developing additional learning scenarios to be evaluated–lab experiments supported by the developed AR training system.

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