MolyPoly: A 3D Immersive Gesture Controlled Approach to Visuo-Spatial Learning of Organic Chemistry

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Abstract. Currently, first-year chemistry students learn about three-dimensional molecular structures using a combination of lectures, tutorials, and practical hands-on experience with molecular chemistry kits. We have developed a basic 3D molecule construction simulation, called *MolyPoly*. The system was designed to augment the teaching of organic chemistry by helping students grasp the concepts of chemistry through visualisation in an immersive environment, 3D natural interaction, and audio lesson feedback. This paper presents the results of a pilot study conducted with a first-year chemistry class at the University of Tasmania. Participating students were split into two groups: *MolyPoly* group (no lecturer in the sessions) and traditional classroom group during the four in-semester classroom sessions over a period of two weeks. We present our comparative analyses over the knowledge-based pretest and posttest of the two groups, by discussing the overall improvement as well as investigating the improvement over the test questions with different knowledge difficulty levels and different required spatial knowledge.

Keywords: Organic chemistry · Gesture controlled · Immersive environment · Visuo-spatial reasoning and learning

1 Introduction

Visual representations and physical models are commonplace in science teaching [1, 2]. One of their applications is to enhance the spatial awareness of concepts [1, 3]. In organic chemistry it is important for students to be able to understand the 3D relationship of the molecules to comprehend concepts such as isomerisation, intermolecular

T. Wyeld et al. (Eds.): OzCHI 2013, LNCS 8433, pp. 153–170, 2015.
DOI: 10.1007/978-3-319-16940-8_8

forces and reaction mechanisms [4, 5]. It has been found that when students understand the 3D spatial arrangement of atoms and molecules, how this relates to the 3D and 2D representations printed in textbooks and how to transpose them into a diagram in order to communicate the particular molecule to another chemist, students do better overall in exam or test results, even when the question does not relate to the shape of the chemical [2]. These results suggest that spatial ability is important for learning scientific topics that involve spatial reasoning.

Indeed, spatial ability, defined by Lohman [6] as "the ability to generate, retain, retrieve, and transform well-structured visual images", has often been considered as an individual difference critical for learning advanced scientific and engineering concepts. For example, a recent longitudinal study [7] showed that spatial ability assessed during adolescence was a salient cognitive attribute among those who subsequently go on to achieve advanced educational credentials and occupations in domains of science, technology, engineering, and mathematics (STEM). Another study [8] showed a web-based virtual environment improved the overall spatial ability focusing on mental rotation and spatial visualization, which provided evidence that spatial ability can be improved through learning environments. Psychological studies have also shown that the ability to perform spatial reasoning and problem solving is critical for predicting performance in a wide range of domains [9–11].

Given its importance, researchers have been evaluating how technologies can be involved in instructional methods to improve spatial ability [12–16]. In particular, interactive 3D environments appear promising to provide the needed tools for spatial ability training. Interactive technologies not only allow students to visualize 2D or abstract elements and relations in 3D, they also allow them to directly manipulate the simulated objects using natural gestures and body movements. These characteristics afford more natural visuospatial reasoning as abstract relations or inferences do not need to be represented and transformed internally as mental imagery [17, 18]. Rather, these relations can be offloaded to perception and action as the learner directly manipulates the 3D simulated objects [19]. Given that external representations of simulated objects are constrained by a medium and unconstrained by working memory, inconsistencies, ambiguities, and incompleteness may be reduced in external representations.

Visuospatial reasoning does not only entail visuospatial transformations on visuospatial information. Visuospatial reasoning also includes making inferences from visuospatial information, whether that information is in the mind or in the world [20]. As cognitive tools, immersive 3D systems facilitate reasoning, both by externalizing, thus offloading memory and processing, and by mapping abstract reasoning onto spatial comparisons and transformations. The systems can organize and schematize spatial and abstract information to highlight and focus the essential information.

In addition to visuospatial reasoning, the interactive nature of these systems allows learners to directly manipulate spatial relations to augment the reasoning process. Interaction of mind and body in reasoning has been revealed when people "interact with virtual objects" in gestures. For example, when people describe space but are asked to sit on their hands to prevent gesturing, their speech falters [21], suggesting that the acts of gesturing promote spatial reasoning. The importance of gestures seems to go beyond manipulation of objects in the external environment, as even blind children

gesture as they describe spatial layouts [22]. These results suggest that gesture controlled systems have the potential to facilitate visuo-spatial reasoning and learning.

To summarize, research shows that immersive interactive systems have great potential to promote visuospatial reasoning by externalizing complex spatial relations and providing interactive tools for direct manipulation of spatial objects. In this paper, we describe the design of such a system called MolyPoly that helps students explore and learn complex spatial relations in organic chemistry.

2 Motivation

To help students comprehend the spatial environment of the molecule, many different models can be used. Originally these were provided in a textbook, which contained 2D diagrams and pictures of 3D molecules in different formats – ball and stick, ball and cylinders and space filling. Limitations of physical models include the amount of sets available, the number of atoms (balls) and bonds (sticks) as well as the types of molecules that can be made [3].

As computers and ease of software development became widespread, so did the availability of computer-generated models of organic molecules. Developments in computer generated molecules range from merely drawing a 2D diagram through to having a rotating 3D model of a molecule. Some of these applications have overcome the limitations of the physical models – not only those listed previously but also the different bond lengths and atoms sizes, which occur within different bonding systems [3, 5]. One of the other difficulties for students is the ability to mentally picture a 3D molecule from a flat (2D) representation.

Although there has been much investment and research into computer simulations to teach science, there is still more work needed before they become commonplace within classrooms, such as the issue of teacher preparedness to utilize a simulation to teach science concepts [23]. Therefore the teaching tools that are commonly used in a university chemistry unit consist of textbook images, 2D diagrams and plastic models (e.g. balls and sticks) for spatial awareness of the molecules' shape. While these low-cost models are economic teaching aids, they often require explicit instruction and guidance from teachers, as the plastic models do not have enough constraints to guide students to create organic structures based on their 2D diagrams. An interactive system, although more expensive, can have built-in constraints and feedback that allow students to explore the mapping between 2D diagrams and 3D structures without much guidance from a teacher. While these systems are not intended to completely replace teachers, they are promising tools that complement regular instructions by allowing students to explore and learn on their own. This paper describes the evaluation of a chemistry teaching system named MolyPoly, designed to facilitate visuo-spatial reasoning and learning for spatial knowledge content. To preview our results, we found that students who used MolyPoly to learn by themselves showed significant learning effects comparable to students who learned under teacher guidance in a traditional classroom using plastic models. However, before we describe details of MolyPoly, we will first review the use of 3D models to teach chemistry.

3 Related Work

3.1 Current State of Molecular Chemistry Teaching

Chemistry teaching is largely about students visualizing and coming to terms with how molecules are arranged and structured as there can be very complicated molecular structures. Visual representations and physical models are commonplace in molecular science teaching [2, 24]. One of their applications is to enhance the spatial awareness of concepts [1].

Being able to visualize and understand the structures in 3D is difficult for the students to achieve, so to help students comprehend the spatial environment of the molecule many different types of representative models can be used. As mentioned earlier, originally these were provided through a textbook with 2D diagrams and pictures of 3D molecules. Today, physical models are used to assist the student with the visualisation of the 3D structures. These models come in a variety of different sizes and are used to let students touch and clearly visualize the structures.

3.2 Issues with Molecular Chemistry Teaching Practices

The aforementioned physical models or molecular model kits (Fig. 1) used by chemistry students to aid visualisation of molecules were previously identified to have limitations [3]. Other issues with the physical models are that they can become difficult to assemble when creating larger structures and that it can be difficult for students to manually check if the structure created was correctly built [25] as opposed to being automatically checked by a computer program.

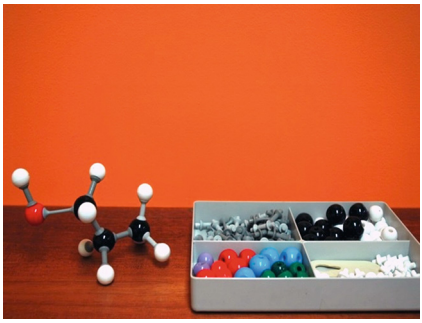


Fig. 1. Molecular **Model kit**

A potential issue with teaching methods may also exist according to Erenay's case study [26], which found that the methods of teaching could make a difference as some approaches can hinder students' exploration into the content. In particular, laboratory work was one such method that can limit exploration into certain topics. In Macgrath's study [27], during a study into teaching students special relativity, demonstrated that due to the nature of special relativity, where studying the effects is quite restricted as

the study of special relativity only becomes significant at near light speeds, making teaching the subject difficult. Therefore, a computer simulation was created that allowed the students to virtually experience recreations without having to abide by "real-world" constraints. Furthermore, computer simulations were suggested by Noeth [28] as a more viable alternative to physical models as it has been shown that using computer technology in schools has helped improve retention, traditional instruction and student learning efficiency, especially for students that are underachieving.

3.3 Immersive Environment Teaching Systems

Development of computer generated molecules stem from just drawing a 2D diagram to having a rotating 3D molecule both of which are viewed on 2D screens. Some of the earlier applications already overcame the limitations of the physical models such as the different bond lengths and atom sizes, which occur within different bonding systems [5].

Apart from molecular chemistry, there are many successful examples where teaching systems have indeed helped improve the learning environment as well as other classroom aspects for students. A particular example is Minimally Invasive Surgical Trainer (MIST), an immersive virtual reality (VR) system used to teach surgeons laparoscopic tasks. It was found that the system helped improve the performance of training surgeons as they were likely to make fewer errors than the surgeons who trained without the simulator [29]. This could be an indicator of the precision consistency of simulators, as these systems or applications can be created to consistently (and repeatedly) deliver the same lesson and experience. Teaching systems can also be based upon existing simulators or video games and repurposed into adaptions that can suit specific purposes. For example, repurposed video games have been demonstrated to maximize learning efficiency and classroom activity [30, 31].

Furthermore, it has been found that virtual environments experienced by the user through VR can be personalized to the individual learner's needs and depending on the environment the learner is free to make a variety of choices. These environments can also help the learner focus on the task at hand instead of being distracted by what is physically around them [32]. In another example, VR teaching systems are being used to train people in other areas, such as occupational health and safety training for carpentry students who were provided with a virtual environment to experience certain situations that happen on a construction site. The study found a high level of user engagement within the educational 3D computer game environment, which was a key factor for the positive learning results. Moreover, carpentry students preferred to learn using the game, with increased content understanding and retention, which can lead to skill sets being considered more relevant [33]. A high level of user engagement is a result of an active learning and constructivist approach when the participants are actively engaged with the content and construct their own knowledge.

Another important benefit demonstrated in some immersive VR teaching systems is the ability to teach students without a teacher needing to be present. This was demonstrated by a recent study into a VR dance training system which used motion capture technology to capture motions from the user and then gave real-time on-screen feedback to the users. The results from their experiment found that participants that used the

system performed better than their control group (learning by watching videos) and that the participants found the method of learning more interesting and highly engaging than simply learning from watching videos [34].

4 Design of *MolyPoly*

MolyPoly is a basic 3D molecule construction simulation, specifically designed to help first-year university chemistry students learn organic chemistry. The organic chemistry requires students to understand the 3D spatial arrangement of atoms and molecules and how this relates to 3D/2D representations in conventional chemistry textbooks. As discussed earlier, an immersive 3D environment is a potential tool for spatial ability training and gesture-controlled systems have potential to facilitate visuo-spatial reasoning and learning. As a result, the first key design of MolyPoly was to combine these two considerations and create an immersive 3D environment that a user (student) can interact with the molecules using their gestures (enabling by a Kinect device).

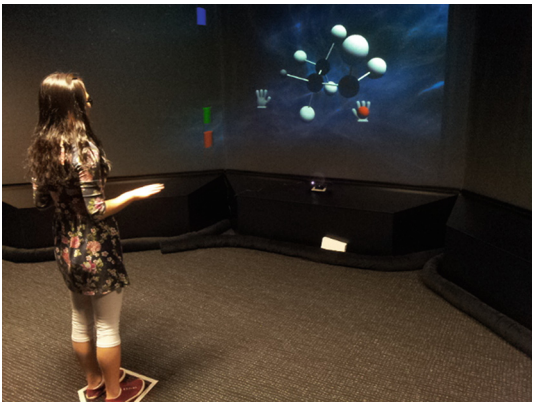


Fig. 2. MolyPoly in use (notice Kinect at the bottom of the middle screen).

Figure 2 shows the system running an immersive 3D environment on three wall-size large displays (the HIT Lab AU's "VisionSpace", wall-size rear projection screens). Furthermore, MolyPoly utilized VisionSpace's 3D stereoscopic capability (passive 3D with polarized glasses) to deliver the immersive 3D environment where users could see the depth inside the molecule structures. The second key design of MolyPoly was to incorporate a built-in lesson feedback that a user can access during lessons. This helps make MolyPoly a self-driven learning tool.

MolyPoly contains five different lessons in which participants used to create five molecular organic structures as illustrated in Fig. 3. Each lesson contains one molecule lesson (Methane, Propane, 1-Propanal, 2-Propanal, Methoxymethane).

A user can engage the built-in lesson feedback during the lessons via a Check-progress virtual bottom inside the 3D environment, see Fig. 5. Once engaged, Moly-Poly will determine the structural correctness of the molecule structure that was

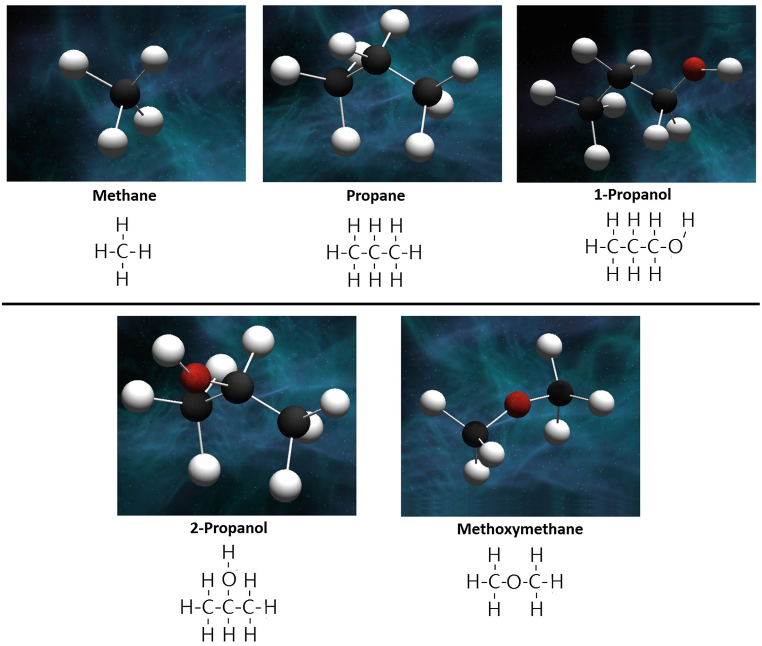


Fig. 3. 3D molecules with the corresponding 2D diagrams (Color figure online).

constructed and subsequentially provide audio and visual feedback as to why the structure is correct or incorrect (e.g., there are not enough carbon molecules). The feedback is determined by an algorithm that runs through a set of conditions that need to be met for that particular molecule (lesson). If all of the conditions are met then the application will provide an on-screen success message, as illustrated in Fig. 4, with a 2D diagram of the structure and make an audible announcement of the success. However, if a mistake was made the system will also inform the user through an audible announcement. In addition, the application will provide audible feedback to let the user know the reason. Due to the simplicity of the lessons in our study, we were able to simplify the condition-checking algorithm to be merely a series of one condition-at-a-time checking and once the fail condition was detected, the algorithm stops and provides the message mostly relevant to the failed condition.

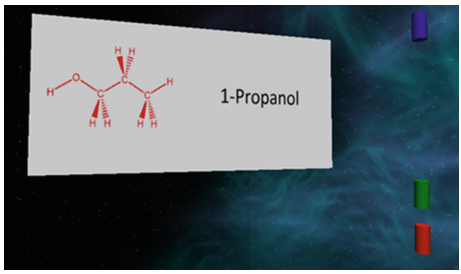


Fig. 4. Visual success message displayed on the left screen of the VisionSpace (Color figure online)

Below is an example of the sequential conditions used in the molecule structure '1-Propanol':

1. Is there one oxygen (red colour ball)?
2. Are there one carbon and one hydrogen connected to one oxygen?
3. Are there a total of three carbons existing in the structure?
4. Are there three hydrogen connected to two carbon?
5. Is there one carbon which has two hydrogen attached?
6. Check that one carbon has two hydrogen, one carbon and oxygen attached.
7. Success message!

4.1 Development of *MolyPoly*

The MolyPoly system was developed in C# using Unity 3D 4 for rapid development. Two Unity plugins were PlayMaker, a visual programming plugin, and a Kinect Wrapper, enabling access to the Kinect SDK. The wrapper is an API that is used to access the functions that are present in the Kinect SDK version 1.7 within Unity. The compiled application interacts with the Kinect wrapper through the code and PlayMaker to get tracking information and access certain hardware functions such as adjusting the Kinect's motor to change the angle and turning the depth sensor on and off, which can be achieved through the Unity GUI as well.

Stereoscopic 3D was enabled by utilizing an adapted Unity 4 camera script written in C# that enabled the application to be viewed in 3D using 3D glasses which allows the users to experience a "pop-out" effect where the molecules feel as if they are coming out of the screen and into physical space. This script was created by the HIT Lab Australia specifically for student projects to utilize the VisionSpace screens' stereoscopic functionality (http://www.hitlab.utas.edu.au/wiki/Stereoscopic_3D).

4.2 Interactions

Gestures were detected through the use of the Kinect skeletal tracking. The skeletal tracking can detect the positions of two hands and in turn, they are represented in the immersive 3D environment as cartoon-style 3D hand avatars, as illustrated in Fig. 5.

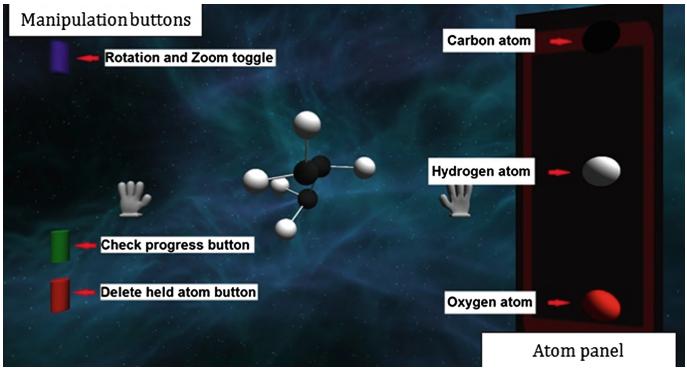


Fig. 5. MolyPoly's immersive workspace with description annotation (Color figure online)

The workspace of MolyPoly is displayed on the VisionSpace projection screens with the molecule structure that is under construction displayed at the center of the workspace and features, which consist of two main control panels: (1) manipulation panel (on the left) and (2) atom selection panel (on the right), as detailed in the following:

Manipulation panel (left side of the application):

- The (top) blue button enables the rotation and zoom.
- The (Second from top) green button gives audible feedback on the correctness of the molecule structure that the user is constructing.
- The (bottom) red button deletes an atom that is currently held in either virtual hand.

Atom panel (right side of the application):

- This area allows the user to pick up carbon, hydrogen or oxygen atoms for connecting with the main structure in the center of the workspace. (Note that only one atom can be held at a time).

All buttons can be activated by simply hovering the virtual hand over them for two seconds (to avoid random hand movements accidentally triggering the buttons). However, the two panels make available two different sets of interaction. The manipulation panel enables users to rotate and scale (zoom) the 3D molecules, while the atom panel enables users to construct the molecules from different atoms. The core of the gestural detection algorithm of MolyPoly is to determine the users' inferred gesture from the position of their detected hands in successive Kinect frames.

Gestures were chosen based upon their ease of use and whether they felt natural. In addition, one of the limitations of the Kinect was the ability to track an individual hand across the crossover workspace (e.g. left hand reach over to the right-handed side of the body): therefore, we designed all interaction to have no crossover and therefore individual hands only operated on their side of the body. During the development and pilot test, we trialed a number of gestures, but some were found too hard to use by the pilot testers. For example, an alternative method of rotation was trialed by simply making the molecule face the direction of the cursor. However, it was not chosen due to lack of control and fine rotations. The eventual gestures were found natural, intuitive and easy to perform. The following paragraphs describe the available gestures in further detail;

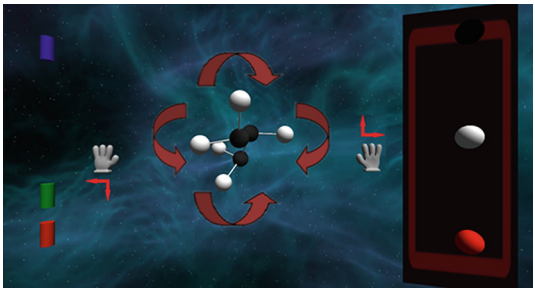


Fig. 6. Workspace with annotated arrows to indicate the directions in which the molecule structure can be rotated.

Rotation. Figure 6 illustrates how the molecular structure can be rotated 360 degrees on the x, y and z axis (note y is vertical axis and x is horizontal axis). The rotation is performed by moving the virtual hands (representing the user's hands) in different directions, as detailed below:

Left hand:

- Move hand down to rotate the structure downward around the x-axis.
- Move hand left to rotate the structure clockwise around the y-axis.

Right hand:

- Move hand up to rotate the structure upwards around the x-axis.
- Move hand right to rotate the structure counter clockwise around the y-axis.

Scale/Zoom. The detection of the zoom gesture was determined by moving both hands either inwards or outwards (in the horizontal axis as illustrated in the top-down view in Fig. 7). A velocity threshold value is used to avoid accidental and unintentional hand movement.

Fig. 7. (Top-down view) Performing the zoom in/out functions. Zooming out by moving both your hands from point 2 to 1 (inwards), while zooming in by moving in the reverse direction from point 1 to 2 (outwards).

Joining Atoms. Atoms can be joined and connected to the molecular structure by picking (selecting) them up and bringing them closer to the main structure. When the atom is in close proximity to another atom that has already been joined and therefore a part of the main molecule structure and still has available link(s), it will display a bond

Fig. 8. Close proximity to the structure displays the available bonds

showing the user that there is an available connection (gray tip in Fig. 8, near the right virtual hand) that can be connected to. The gray tip will change to a red tip when the user moves the selected atom very close to the tip and if the bond's tip stays red for three seconds, the held atom will be bonded (jointed) to the main molecular structure.

5 Experiment

To the authors' knowledge, there has been no research conducted explicitly exploring the effect of using an immersive 3D environment with gesture control on conceptual understanding of foundational chemistry. The aim of our pilot study is to determine whether or not the concept of the MolyPoly's 3D immersive gesture controlled interface can be utilized as an effective teaching tool within the field of chemistry by demonstrating that this technology has the potential to yield beneficial learning outcomes comparable to a traditional teaching method.

The experiment consisted of four sessions over two weeks. Seventeen (17) students from a first-year chemistry class at the University of Tasmania took part in the study. The participants were divided into two groups, MolyPoly and the traditional classroom group based on their scores in a pretest such that the two groups had similar ranges of students' prior subject knowledge. The traditional group of students remained with their normal chemistry classes and created molecular models using physical molecular model kits, whereas the MolyPoly group studied in the HIT Lab AU's VisionSpace, where they used the MolyPoly system to visualize and create molecular structures in conjunction with the printed handout of the lessons, which was used by both groups.

The pretest was conducted to ascertain prior knowledge in order to get a baseline for comparison with posttest after the lessons. The pretest and posttests were identical and consisted of basic chemistry knowledge-based questions, mainly on molecular structure. In the subsequent two weeks, four sessions with five molecular structures were taught to both groups separately using the two different pedagogies.

In the first session, participants selected for the MolyPoly group were shown how to interact with the application so that they had an opportunity to get acquainted with the system. Then, participants were asked to create a simple molecule structure, Methane, while participants in the traditional group were given a traditional lecture about the same structure. During the second session, all participants were required to create Propane, which is a more complex molecule structure. In the third session (second week), 1-Propanol was used in the third session, where the participants were instructed to complete the 1-Propanol structure and upon successful completion they were then able to view a completed 2-Propanol structure for comparison. In the (last) fourth session they were instructed to complete a Methoxymethane model. After all participants had completed the lesson, both groups undertook the posttest.

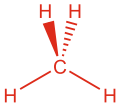
5.1 Pretest and Posttest Questions

Students responded to 15 questions on a pretest/posttest evaluation designed to elicit their conceptual understanding of foundational chemistry. These questions were categorized

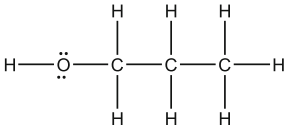
by level of difficulty (easy, moderate, difficult) and by level of required spatial knowledge (none, low, high). Each difficult level contained five questions. There were two questions with non-required spatial knowledge and both were in the easy difficulty level. There were four questions with low-level spatial knowledge with two in the easy difficulty level and two in the moderate difficulty level. The questions with requirement of high-level spatial knowledge contained nine questions that were equally divided across all levels of difficulties (three in each). In summary, the five easy questions required either high spatial knowledge or no spatial knowledge. The five moderate questions required some spatial knowledge (either low or high). Similarly, the five difficult questions required either low or high spatial knowledge.

Example questions are listed below (answers are highlighted in red and in the line immediately below the question line):

- [Easy, High Spatial Knowledge] Draw the full 3D structure for CH_4.



- [Easy, No Spatial Knowledge] The following Lewis Dot Diagram represents Propan-1-ol.



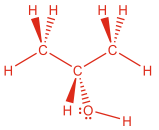
What type of hybridization does the oxygen atom have?

sp^3

- [Medium, Low Spatial Knowledge] Why would Propane have a lower boiling point compared to 1-Propanol?

1-Propanol is able to easily form H-bonding and dispersion forces between molecules whereas Propane is only able to form dispersion forces between molecules.

- [Medium, High Spatial Knowledge] Draw the full 3D structure for propan-2-ol.



- [Difficult, High Spatial Knowledge] Put the following molecules in increasing order according to their boiling point. CH_3CH_3OH, $CH_3CH_2CH_2OH$, and $(CH_3)_2CH_2OH$.

3, 2, 1

At the end of the MolyPoly group experiment, participants were asked to fill in a questionnaire to rate their experience of using the MolyPoly application. There were three main questions: (1) rotation gestures easy to use, (2) zoom gestures easy to use and (3) gestural manipulation improve understanding of the molecular structures. The answers were Likert-scale with 1 Strongly Disagree, 2 Disagree, 3 Neutral, 4 Agree, and 5 Strongly Agree.

5.2 Analysis Strategy

All tests were scored by a member of the research team, who was the subject domain expert and a regular lecturer for the unit. Each question was marked as either right or wrong. All correct responses were tallied to provide the dependent variables for inferential analyses between the two groups (traditional and MolyPoly) and the pretest and posttest. The reliability of this analysis was strengthened by the collaborative marking effort that provided for a moderation process to resolve any conflicting interpretations.

A 2 (group) × 2 (test) mixed design ANOVA, with an alpha level set at 0.05, was used to test for any significant differences between the summative scores of the 15 questions. This was followed by a series six 2 (group) × 2 (test) mixed design ANOVAs to test for significant differences of the summative scores for each of the question difficulty levels ((5) easy, (5) medium, (5) difficult) and level of spatial knowledge ((2) none, (4) low, (9) high) individually. Since several statistical tests were performed, a modified Bonferroni adjustment was applied to the overall critical alpha level before any significant differences were identified. Only statistically significant findings are reported below. All statistical analysis was conducted with SPSS version 22.0.

5.3 Results

There were no statistical differences between the two groups on the pretest evaluation. Both groups improved their foundational knowledge of chemistry over the experimental period. Our analysis indicated that both groups improved their pretest/posttest performance similarly across all question difficulties. There was a statistically significant improvement for the easy and moderate questions, however there was no statistically significant improvement for the difficult questions. There was a statistically significant improvement for the low and high spatial knowledge questions; however, there was no statistically significant improvement for the two questions that contained no spatial knowledge. In summary, one group did not perform better or worse compared to the other group for any of the pretest/posttest comparisons. The details of our significant findings are described in the following paragraph.

The overall analysis of the total 15 questions revealed a significant main effect for test, $F(1,16) = 110.03$, $p = 0.001$. Both groups significantly improved from pretest ($M = 5 \pm 1$) to posttest ($M = 10 \pm 2$), total score of 15. When categorized by level of difficulty, analysing the five easy questions showed there was a significant main effect for test, $F(1,16) = 95.31$, $p = 0.001$. Both groups significantly improved from pretest ($M = 2 \pm 1$) to posttest ($M = 4 \pm 1$). For the five moderate questions, there was a significant main effect for test, $F(1,16) = 32.82$, $p = 0.001$. Both groups significantly improved from pretest ($M = 1 \pm 1$) to posttest ($M = 3 \pm 1$); and for the five difficult questions, there was no significant findings for the improvements noted by both groups, pretest ($M = 2 \pm 1$) to posttest ($M = 2.5 \pm 1$).

For the four questions that required low spatial knowledge, there was a significant main effect for test, $F(1,16) = 22.94$, $p = 0.001$. Both groups significantly improved from pretest ($M = 2 \pm 1$) to posttest ($M = 3 \pm 1$). For the nine questions that require high

spatial knowledge, there was also a significant main effect for test, $F(1,16) = 52.07$, $p = 0.001$. Both groups significantly improved from pretest ($M = 2 \pm 1$) to posttest ($M = 5 \pm 2$).

The time durations in which both groups were working with their respective 3D molecular forms (traditional group–molecular model kit in Fig. 1, MolyPoly group – 3D molecular models in Fig. 3) in each of the lessons were on the average 4.71 min per lesson per group class, across all five lessons, for the traditional classroom group and 2.94 min per lesson per person for the MolyPoly group. The small difference in these exposure times that individuals spent on 3D models were not significant in the context of this study as the small differences were expected due to non-identical teaching pedagogies of the two groups. For the rest of the time (50-min teaching session), the traditional group would go through (typical) passive learning (with and without the use of the model kit) on the printed out lesson materials and Q&A without the use of the model kits. Simpler for the MolyPoly group, students on their own spent the rest of the time learning from the printed out lesson materials, which are the same materials used in the classroom group. As opposed to a traditional group's teacher-driven teaching session, the MolyPoly group environment facilitated student-driven learning or self-direct learning.

The post experiment questionnaire revealed that participants felt more comfortable using Zoom gestures (with an average response of 4.14) than using Rotation gestures (with an average response of 3.14). Furthermore, participants generally agreed that the ability to manipulate the molecular structures in 3D (through MolyPoly) helped them improve their understanding of the structures (with an average response of 3.85).

6 Discussion

Our results showed that the 3D immersive virtual environment created by MolyPoly produced posttest score results comparable to posttest score results of the group with the traditional teaching method. This implied that the use of MolyPoly's 3D immersive gesture controlled interface was as effective as the use of the physical model kits in the spatial learning context. The learning outcomes of the MolyPoly group were results from a combination of using 3D immersive gesture controlled approach and self-direct active learning approach.

MolyPoly's interactive 3D immersive gesture controlled approach has built-in constraints and feedback that allow students to explore the mapping between 2D diagrams and 3D structures. Students were able to use gestures to control the viewpoint of the 3D Molecule structures; spin the molecule to the left, right, up, and down, and additionally zoom in and out of the structures. Combining the gestural control with 3D immersive capabilities created a learning environment that facilitated visuo-spatial reasoning and learning thorough the active learning and constructivist approach. Students were able to actively map what they learned from the lesson information sheets (2D diagram) to their spatial understanding of the 3D molecule structures through the process of constructing those molecules atom-by-atom in a 3D structural manner. Initially, the students had trouble performing the gestures, but they eventually became quite adept at using them effectively following the first lesson. However, as the post

experiment questionnaire revealed, participants found rotation gestures more difficult to use than zoom gestures. The design of the rotation gestures required some cognitive load to operate the two-hands gestures properly; while the inwards and outwards of the zoom gestures were more natural. However, it is worth mentioned that despite some less than natural interaction of our gestures, participants still felt that their ability to manipulate the 3D molecular structures helped them improve their understanding of the molecules. The future work should include the redesign of the gesture interaction that would improve the naturalness of the interaction.

With MolyPoly's in-built lesson feedback, there was no need for a chemistry teacher. This allowed the students to create their own knowledge based on an engaging, meaningful experience. In a traditional teaching method (i.e. classroom), the chemistry teacher often directed the student attention to the "right answer" or informed them what was important to attend to. In the MolyPoly (i.e. self-direct), the students were forced to become active participants in constructing their own learning, allowing them to proceed at their own pace to forge their own conclusions and knowledge. This self-directed active learning style was also evident by the utilisation of the in-built lesson feedback which was used by students in the MolyPoly group on average of 1–3 times per lesson, whereas the traditional classroom group had virtually no direct questions from students during classes. This was most likely attributed to the capacity of MolyPoly to provide real-time, user-initiated augmented feedback that could be elicited as often as requested by each participant within this group. This functionality created by the immersive software environment allowed for more student-driven, individualized, problem-based learning experiences during the intervention period; whereas the traditional group relied on a typical teacher-driven learning experience that did not cater for individual rates of learner progress. Student-centered approaches to learning have often produced better-quality outcomes compared to traditional teacher-centered instructional approaches. For example McDonnell [35] found that chemistry students had a much more engaging learning experience when involved in a 'unique' project, as opposed to the traditional laboratory approach. In Chan's study [34], the participants found learning a dance lesson with a motion-controlled VR dance training system with real-time on-screen feedback much more interesting and highly engaging than simply learning from watching videos.

We believe that if our experiment was replicated across a larger group of students over a longer experiment period, the greater power elicited would demonstrate that the MolyPoly teaching environment would yield better learning outcomes compared to the more traditional teaching environment conducted for introductory level chemistry classes. Furthermore, it was the aim of the researchers to test the amount of learning gained through a 15 question posttest. It would be advantageous for future related research studies to incorporate a retention test so true learning using this technology can be measured.

Our results also implied that the MolyPoly teaching environment has the potential to be a viable teaching solution for remote delivery of knowledge subjects that requires not only spatial reasoning and learning but also self-directed active learning. Future research should explore the possibility of this potential by conducting a field study with real remote classrooms. The un-joining function should also be implemented in the future work so that students can undo the unwanted joining.

7 Conclusions

MolyPoly is a proof of concept of a basic 3D molecule construction simulator, specifically designed to help first-year university chemistry students learn organic chemistry. It was designed to utilize a mixed approach of 3D immersive gesture controlled and self-directed active learning to facilitate visuospatial learning of organic chemistry. The aim of the research was to determine through a pilot study whether MolyPoly could be used as an effective teaching tool for teaching organic chemistry. A pilot study was designed and conducted to compare the comparative learning outcomes between the group which learned with MolyPoly and the group which learned in a traditional classroom. The analyses of the pilot study provided strong evidence that students who learned using MolyPoly demonstrated a pretest-posttest score improvement of learning outcomes comparable to students that learned in traditional classroom.

Comparing the pretest/posttest over different difficulty levels of organic chemistry suggested that the students in the MolyPoly group performed on the tests just as well as the students in the traditional classroom group. Additionally, the two groups performed similarly on the questions, which required different levels (no, low, and high) of spatial knowledge. This is a further indication that the MolyPoly has potential as a teaching tool for the subjects that require spatial reasoning and learning such as organic chemistry.

MolyPoly's 3D immersive environment with gestural controls created the learning environment that promoted visuo-spatial reasoning by externalizing complex spatial relations and providing interactive gesture controlled tools for direct manipulation of spatial relations. Furthermore, MolyPoly's in-built lesson feedback facilitated the self-directed active learning, which promoted active students' engagement in constructing their own learning. This further improved the students' understanding of the subject materials.

Acknowledgements. We would like to acknowledge the support of a Provost Visiting Scholars Program at the University of Tasmania that enabled us to form an international research team. We also would like to acknowledge the contribution of an undergraduate final year project team, MolyMod, who in 2012 helped create the motivation and original conceptual prototype upon which this project was built and Jonathan O'Duffy of the HIT Lab AU for his help during the initial development of MolyPoly in 2013.

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