MolecuSense: Using Force-Feedback Gloves for Creating and Interacting with Ball-and-Stick Molecules in VR

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ABSTRACT

We contribute MolecuSense, a virtual version of a physical molecule construction kit, based on visualization in Virtual Reality (VR) and interaction with force-feedback gloves. Targeting at chemistry education, our goal is to make virtual molecule structures more tangible. Results of an initial user study indicate that the VR molecular construction kit was positively received. Compared to a physical construction kit, the VR molecular construction kit is on the same level in terms of natural interaction. Besides, it fosters the typical digital advantages though, such as saving, exporting, and sharing of molecules. Feedback from the study participants has also revealed potential future avenues for tangible molecule visualizations.

CCS CONCEPTS

• **Human-centered computing** → **Virtual reality**; • **Applied computing** → **Chemistry**.

KEYWORDS

Virtual reality, digital gloves, human-computer interaction

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1 INTRODUCTION

3D models of molecules play a fundamental role in chemistry, both in chemical education and in the frontier research, as the spacial structures significantly aid the understanding of molecular reactivity and properties. Traditionally, in the pre-digital ages, physical models, often implemented as ball-and-stick models, have been used extensively. In the recent two decades, this way of representing molecular models was more and more superseded by computer graphics approaches.

Nevertheless, the traditional physical model bears a lot of advantages, being literally more tangible and offering direct structural manipulations like rotations around bonds which in a natural way allow to explore the conformational space of the molecules. On the other hand, the physical models have some limitations, they become fragile and hard to handle at some larger scale, are difficult to store, to replicate or to share over large distances. On the contrary, the molecular construction software can avoid these disadvantages, and allow to precisely manipulate the position and conformation of the atom cluster to create the structures that are more in line with expectations.

However, mouse-based interaction and the 2D screens might hinder spatial and haptic thinking in 3D molecular construction tasks.

Ideally, we would like to get a tool, that combines the benefits of these two approaches, by combining tangible experience creating these models with the digital amenities. In collaboration with chemistry researchers, we thus decided to set out to explore how Virtual Reality (VR) and force-feedback gloves could be used as an alternative for creating and interacting with ball-and-stick molecules.

To test this idea, we built a VR-based prototype using the HTC VIVE for output, and force-feedback SenseGlove[1]s as input. The SenseGloves enable users to grasp virtual objects by controlling motors on the finger joints and thus have the potential to offer a better presence than ordinary VR controllers [11]. The existing works have shown that offering such force-feedback could make for an increased usability and user experience when using molecular visualization tools [3, 10, 12, 20].

We see the main novelty of our work lies in the careful combination of molecular construction and force feedback for grasping, holding, and manipulating in virtual reality. In summary, our work makes the following contributions:

- The design and implementation of the MolecuSense prototype, that leverages VR and force-feedback.
- A preliminary usability evaluation of MolecuSense, revealing some insights into the usage of modern force-feedback gloves for virtual ball-and-stick molecules.

2 BACKGROUND AND RELATED WORK

In addition to the classic molecular construction kits, in which users assemble the parts by hand, there are now also some computer programs for modelling molecules. With these programs, not only simple molecules can be formed, but far more complex calculations and visualizations can be done depending on the focus. Avogadro [8], for example, an open source program, supports the dynamic loading of plug-ins and can therefore always be expanded, so that new types of visualization can be viewed. Whereas traditional molecular visualizers show molecules in front of you, Molecular Rift, a VR molecule construction kit presented by Norrby et al. [13],

[1]https://www.senseglove.com/

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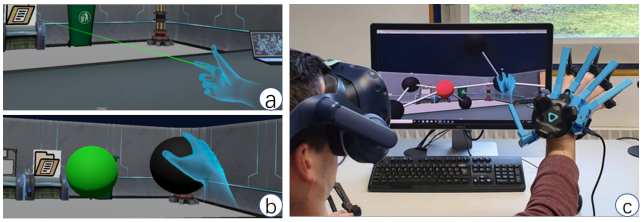

Figure 1: (a) The pointing gesture for operating all basic functions of the program. (b) The users can hold an atom by the grasping gesture. When two atoms are close enough, the unheld one will flash in green, indicating that the current distance can form a bond. (c) This is an example of using MolecuSense for VR.

lets the user enter the the interior of molecules and explore the unique and realistic 3D effects offered by the VR. They developed a gesture-controlled VR program to easily create molecules for drugs development, which demonstrates its potential when investigating various molecular systems, and received very positive feedback from several focus groups.

One possibility to increase immersion in VR systems is the integration of haptic feedback. According to Ramsamy et al. [15], presence and efficiency are increased when users can feel and touch virtual objects. The means used to generate haptic feedback range from devices placed on fingertips to exoskeletal gloves. Exoskeletal gloves, such as the SenseGlove used in our study, cannot give a feeling about the mass of the virtual objects, but it enables the users to perceive the shape of virtual objects. The SoftGlove [18], a further development of the SenseGlove, contains an exoskeleton that lies over the hand and a size-adjustable glove with vibration motors attached to it to improve the force feedback, i.e. the forces acting on the individual fingers and the fit. In addition, more stable fingertip caps have been added to distribute the pressure evenly. This prototype shows that immersion in VR can be improved by haptic feedback, but also needs to be refined in many areas.

Most closely related to our work are approaches that seek to incorporate haptic and force feedback into the construction of molecules. Historical endeavors into that direction used mostly hand-grasped, stylus-based, grounded devices [16]. Such approaches were found to potentially enhance the spatial visualization [20]. Besides, such haptic devices might provide force-torque feedback [10], and amplify the atomic force in the molecular environment for better perception, and eventually help the users find the best docking position [3, 12]. In MolecuSense, we expand this line of research by looking at modern force-feedback gloves as an input and output device, which provides a physical perception about the shape of atoms and molecules.

3 PROTOTYPICAL DESIGN

For MolecuSense, we seek to combine digital amenities with the tangible experience of molecule construction. To address that, we visualize the atoms and their chemical bonds with a traditional ball-and-stick model [21] in VR. The force-feedback gloves are used to interactively generate and manipulate the molecule models.

3.1 Design Principles and Requirements

A molecule visualized in the ball-and-stick model consists of atoms (balls) and bonds (sticks) connecting them. The chemical element of each atom is indicated by the ball's color and size; an example is shown in Figure 1(b). The angles between sticks on the same atom should be identical to the bond angles. Abstractly, we can think of such models as a constrained 3D node-link diagram.

Existing graphical user interface of digital tools, such as TmoleX [6, 19] and Avogadro [8], have sought to re-use this ball-and-stick metaphor. By analyzing physical and digital tools, we have summarized a list of basic tasks to interact with ball-and-stick models:

- **T1**. Creating/removing an atom.
- **T2**. Constructing a molecule by linking the atoms.
- **T3**. Moving/rotating a molecule.
- **T4**. Editing an existing molecule via an operation panel.
- **T5**. Saving/loading a molecule.

3.2 Visual Design

In MolecuSense, the atoms are represented by 3D spheres and chemical bonds by sticks, just as in the real physical model. For each atom, we reserved a certain number of vacancies to build bonds, according to the chemical valencies of that atom, which is its capability of forming a certain number of chemical bonds, for instance, four for Carbon and one for Hydrogen. For the atom with multiple vacancies, we preset the position of each vacancy on its surface, to ensure that the single bonds (sticks) connected to this atom form a stable symmetric structure, such as the tetrahedral molecular geometry of Methane (CH_4).

In this paper, we focus on Carbon atoms with single chemical bonds for illustrative purposes.

3.3 Construction of molecules

To support the tasks outlined above, we designed two gestures and one additional mode for users to construct molecules.

(1) Pointing gesture. The virtual pointer has been widely used in distant selection in virtual reality, for instance, gaze [23] and ray emitted from hand-held controllers. In MolecuSense, we follow this technique and realize it by pointing gesture. When a user makes a "finger gun" gesture, the index finger will emit a ray (Figure 1(a)). To select a target, the user needs to press the thumb towards the index finger. This gesture can be used to click on distant buttons, whose functions include creating/deleting an atom (**T1**) or opening the folder to save/load (**T5**) a molecule structure. In addition, when saving a molecular structure, we encoded the position and connection data of the atoms into an XML file [4].

(2) Grasping gesture. The most natural way to interact with 3D objects in virtual environments is to use humans hands [24], which can be supported by force-feedback gloves. In MolecuSense, users can manipulate a molecule by grasping any atom in the molecule, including movement and rotation (**T3**). The atoms and molecules with electron vacancies can be joined together via drag-and-drop. When a user holds an atom close to an existing atom or molecule and reaches a distance threshold, the existing one will flash, as seen in Figure 1(b). In this case, once the user releases the gesture, the chemical bond represented by a default-length stick will link these two structures (**T2**).

(3) Edit mode. When using the pointing gesture to select an atom in an existing molecule, the edit mode will be activated/deactivated. In this mode, the selected atom is marked red and frozen in space, and the angles of all bonds connected to this atom will be presented (Figure 1(c)). The user can manipulate the other atoms via the grasping gesture, to changes the length and angles of bonds, which can even be used to construct ring structures (**T4**). After releasing the grasping gesture, all unselected atoms will be slightly adjusted in position based on a simple molecular force field with interatomic spring forces.

In this study we implemented MolecuSense in a virtual laboratory developed with Unity 3D, and used a HTC VIVE Pro set, which consists of a HMD, two base stations, and two 6-DOF trackers on a pair of SenseGloves (Figure 1 (c)).

4 USER STUDY

We designed MolecuSense to combine the advantages of digitization and tactile interaction in VR. To verify this, we conducted a user study to compare MolecuSense with existing molecular construction tools that have only one of the above advantages: a PC-based tool, which provides digital amenities, and a physical ball-and-stick construction kit. While we did not have available a stylus-based haptic device [3], studying the differences between different haptic devices would be similarly interesting and poses fruitful avenues for future work.

4.1 Study Design & Hypotheses

A total of 18 people at the local university participated in this study, aged 19-39 years (13 males & 5 females). 12 of them majored in chemistry, while the others had basic school knowledge of chemistry (Non-chemistry). We conducted our study as a within-subject design, with Tool (VR, PC, physical model (PHY)) as the sole factor. Based on the tasks proposed in Section 3.1, we chose TmoleX[2] [6, 19] for the PC condition and prepared an Orbit molecular model kit[3] for the PHY condition. Both tools are also based on the ball-and-stick model. We let the subjects perform a molecule construction task involving carbon atoms, and measured the workload with a questionnaire and task completion time, as well as the usability of different tools.

We formulated two hypotheses for the experiment:

- **H1**. VR and PHY will cause less workload than PC.
- **H2**. There is no significant difference between VR and PHY in terms of the system usability.

4.2 Procedure & Task

Participants read the study description, and then completed the form of consent and a demographic questionnaire. The participants needed to use different tools to perform the same task. To avoid order effects, we used a Latin Square to counterbalance the order of the tools. The task consisted of the following sequence of steps:

(1) Create the carbon skeleton of 2-methylbutane.
(2) In edit mode, rotate the individual methyl groups in 2-methylbutane into another conformation.
(3) Delete / disassemble the molecule.
(4) Load the prefabricated carbon skeleton of cyclopentane.
(5) Delete at least one atom of cyclopentane and then use the rest to create the carbon skeleton of norbornane.
(6) Save the molecule (only in VR and PC).

After each session, the participants were asked to complete the NASA Task Load Index (TLX) [9] and the System Usability Scale (SUS) [2] based on the experience about the current tool. For our VR-based tool, the participants filled also a presence questionnaire [22]. And for each tool, we recorded the total time that the participants spent on completing the task. After all sessions, we conducted a semi-open interview on subjective preferences and experiences using the different conditions.

4.3 Results

For statistical analysis, we first ran the Shapiro Wilk's test [17] and confirmed the normality of dependent variables ($p \geq 0.05$). The Welch Two Sample t-test showed no significant difference for Expertise between chemistry and Non-chemistry(t=-1.3903, p=0.174). We therefore combine the data and reanalyzed it using One-Way Repeated Measures ANOVA, with Tool as the only factor. For statistical analyses, we first ran the Shapiro Wilk's test [17] for normality of dependent variables. Then we used Greenhous-Geisser corrections [7] to adjust the lack of sphericity and reported effect sizes with generalized Eta squared (η^2_G) for ANOVA [1]. For post-hoc tests, we tested the hypotheses with 95% confidence interval (CI) and visualized them respectively [5]. For statistical p-values greater than or equal to 0.001, we report their exact values; for the ones less than 0.001 we report them as "p<.001".

Completion Time & Workload. As can be seen in Figure 2 (a), there is a significantly statistical main effect of Tool on completion time ($F_{2,34}$=67.863, p<.001, η^2_G=.643). Overall, PHY had a consistently lower completion time than VR (t=6.61, p<.001) and PC (t=9.08, p<.001). The completion time for VR was significantly lower than PC (t=3.98, p<.001).

The result of TLX questionnaire showed the same situation (Figure 2 (b)), that the significant main effect was found for Tool ($F_{2,34}$=46.718, p<.001, η^2_G=.376). PC had a consistently higher TLX score than PHY (t=5.343, p<.001) and VR (t=3.99, p<.001). The TLX score for VR was trending higher than PHY (t=1.31, p=.20).

System Usability. According to the result of SUS, the system usability was affected significantly by Tool ($F_{2,34}$=110.66, p<.001, η^2_G=.794). As seen in Figure 2 (c), PC had consistently lower SUS scores than VR (t=11.008, p=<.001) and PHY (t=11.94, p<.001). And the SUS score for VR was sightly lower than PHY (t=0.66, p=.51).

Presence. We assessed the presence of MolecuSence with the average values of the presence questionnaire. As shown in Figure 3, we also compared the subscales of the questionnaire with the standard values provided by UQO Cyberpsychological Laboratory: (a) Realism, (b) Possibility to act, (c) Quality of Interface, (d) Possibility to examine, and (e) Self-evaluation of performance. Although we do not have the complete dataset for the standard level, it can still roughly be observed, that MolecuSense had higher scores for all subscales than standard level.

Subjective Feedback. According to the semi-open interviews, 16 out of 18 participants preferred VR compared to the other two tools.

[2]https://tmolex.software.informer.com/
[3]https://bit.ly/3uBjKiU

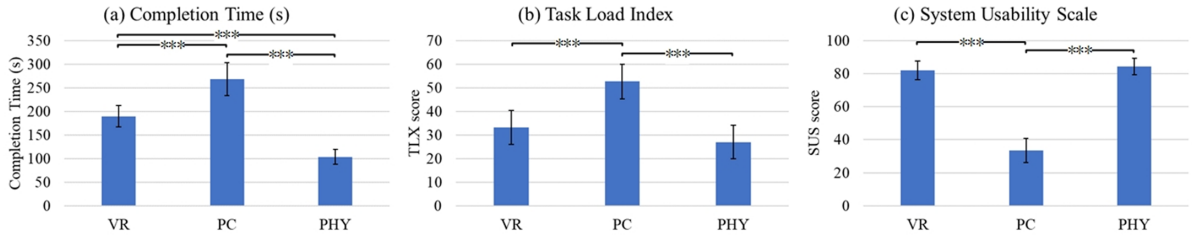

Figure 2: Overview of the results of user study. (a) Completion time: PHY <VR <PC. (b) TLX: PHY <PC & VR <PC. (c) System Usability: PC <VR & PC <PHY. The significant differences have been marked with stars * (* for p<.05, ** for p<.01, and * for p<.001). The error bars denote the 95% confidence intervals.**

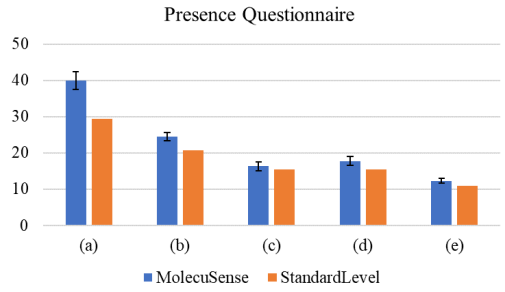

Figure 3: The average values of Presence questionnaire. Error bars show 95% CIs. (a) Realism. (b) Possibility to act. (c) Quality of Interface. (d) Possibility to examine. (e) Self-evaluation of performance.

The remaining two participants both have professional backgrounds in chemistry. One of them chose PC and the other preferred PHY, because they used the corresponding tools frequently in daily work.

5 DISCUSSION

The study results preliminarily support our hypotheses H1 and H2.

H1 accepted: Both PHY and VR had lower values than PC in terms of completion time and TLX scale, which supports that these tools caused less workload. According to the subjective feedback, the interactive way of constructing a model by hand felt natural and intuitive, which evoked less mental and temporal demand.

H2 accepted: We did not find a significant difference between VR and PHY in terms of SUS. Since we take PHY condition as an example of tangible molecule construction, and that VR condition meets the standard levels on most subscales of presence questionnaire, we think this provides evidence that MolecuSense might inherit the advantages of tactile feedback from physical models. Note, that of course with the statistical framework taken, we can never fully prove such a statement.

6 LIMITATIONS & FUTURE WORK

This research has limitations regarding prototype and user study. Many users reported that technical flaws of SenseGlove increased the difficulty of the tasks, although MolecuSense was able to satisfy the basic needs for preliminary construction. For example, the fingertips of the virtual hand did not completely correspond to the real finger, which took the participants more time to perform the gestures. In addition, the inaccuracy of force feedback in some places made the participants miss the best positions, which together with the cable in the glove limited the finger movements.

In terms of evaluation, we only measured the holistic completion time under each condition, so we did not compare the impact of each tool on different sub-tasks. Future work might also break it down into the time metrics for individual tasks. Besides, we did not include other objective metrics, such as the count of errors when performing sub-tasks. We found that creating a fair error metric is non-trivial, especially under the physical-model condition, in which the participants' errors could only be subjectively perceived by themselves.

Although we found initial evidence toward our hypotheses, the molecule construction task in our experiment were relatively simple and only involved Carbon atoms. With more types of atoms and more complex structures involved, the usability and workload of MolecuSense might change.

7 CONCLUSION

. In this paper, we presented MolecuSense, a VR-based molecule construction tool. This tool combines the advantages of digital amenities and tactile experience, by allowing users to use force-feedback gloves to manipulate atoms, build bonds, and eventually construct molecules, as well as saving and loading molecule structures. A preliminary study was conducted to compare its workload and usability with existing tools. The results showed that while this VR-based molecular construction kit retains some advantages of digitization, it is closer to the physical models in terms of natural interaction than PC-based tools. We hope that our work on MolecuSense will inspire other researcher towards using new forms of interaction for visualization, and by doing so get closer toward the much needed "science of interaction" for visualization [14].

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