MR. Mol: Mixed Reality Molecule

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INTRODUCTION AND PURPOSE

Our research group, inspired by an augmented reality (AR) experiment created by the Georgia Gwinnett College (GGC) Chemistry Department, has partnered with GGC faculty in an interdisciplinary effort to create an application that allows the user to manipulate and simultaneously compare molecules projected by the Microsoft HoloLens, a mixed reality (MR) device. Our program builds on and improves an initial AR effort that combined smartphones, tablets, and Aurasma to convert a 2D molecule structure drawn on paper into a 3D object, enabling the user to interact with the molecule on their device (1). While the initial experiment allows for active learning, there are restrictions such as having to hold the device over the 2D drawing to view the 3D molecules in Aurasma. Viewing capacity is also limited to the size of the device screen. Instead of pursuing an AR learning environment, our team has decided to take it a step further and provide a fully interactive MR learning experience for the user via the Microsoft HoloLens headset.

Our team is pursuing the simulation of a kinesthetic learning experience for studying molecules in the classroom. MR brings a sense of realness to an otherwise impalpable object. Students can have a simulated hands-on learning experience with objects that are typically limited to 2D. The 3D nature of molecular structures has a dramatic impact on their chemical and physical properties. Many molecular structures have complex characteristics that are lost when represented in a 2D form. When students are unable to visualize the 2D representations of molecules in 3D, they struggle to understand molecular properties and concepts such as stereochemistry. MR fortifies learning by removing the constraints of working with a flat projection and offers an engaging platform to challenge how students and educators alike interact with molecular visualizations (2). In our case, users can omni-directionally study a molecule and even compare molecules, allowing for a deeper comprehension and understanding of the molecules' physical composition and chemical interactions. The holographic model has differentiating advantages over tactile learning tools, like plastic molecular model kits, because molecular structures can be preloaded and do not have to be put together manually. The ability to scale gives users various accurate perspectives and details of particularly complex structures.

PROOF OF CONCEPT

The proof of concept is a prototype application that allows for the manipulation of molecules projected by the Microsoft HoloLens. The custom HoloLens application displays molecular structures in a mixed reality environment, allowing the user to maneuver (select, move, scale, and rotate) and compare two molecules simultaneously. The user can even “walk around” the molecule if they desire while combining gaze, voice and gesture commands.

HARDWARE AND SOFTWARE IMPLEMENTATION

Mixed reality (MR) is a blend of the real world and the virtual world in which physical and digital objects exist and interact in real time. With the rise of interactive technology, many acquisition devices have been introduced which allow the user to control the device without touching the keyboard, the mouse, or the screen (3). Devices like the Microsoft HoloLens "break down the barriers between virtual and physical reality, and enable the physical and virtual worlds to intersect in new ways" (4). Instead of either being completely cut off from the outside world, as with virtual reality (VR), or being confined to viewing a 3D object on a screen, as with augmented reality (AR), MR provides an immersive experience that merges holograms into the user's physical environment while allowing the high-quality holographs to be viewed from all directions (2, 4). The HoloLens is a self-contained system that generates and projects stereographic images onto the lenses of a headset (4). In addition to having a central processing unit, the HoloLens contains a separate holographic processing unit that allows 3D graphics to exist in the user's physical space while keeping track of user input such as voice commands and gestures (4). Because the HoloLens uses tracking that combines data from multiple input sensors and cameras with algorithms, the device is able render a smooth MR experience (5).

We are implementing the use of the Microsoft HoloLens and the Unity Game Development Engine in order to develop directly into the HoloLens. Our program allows a user to select two molecules to examine and compare as needed from a list. Once selected, the molecule is displayed. Molecule data is retrieved from the PubChem website (6) and procedurally built as a hologram. Using a combination of gaze, voice, and gesture controls, users can select, reposition, rotate, scale, and reset the molecular structures, via selecting from the menu or via voice command, to get a better understanding of their characteristics. Figure 1 to the above shows a snapshot of our application's user interface, and Figure 2 below shows the application workflow.

Figure 1

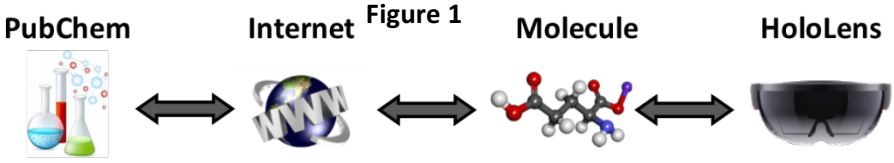

Figure 2

CONCLUSION

Mixed reality (MR) creates an immersive environment with virtual objects inlaid into the real world. This interactive setting is optimal for exploring the intricate 3D characteristics of molecular structures. The use of gaze, voice, and gesture controls allow for easy manipulation of the holographic molecules. Combined, these features enhance both teaching and learning by bringing otherwise 2D objects to life.

REFERENCES

1. Pennington, Richard, Behmke, Derek & Lutz, Robert (2016, 24 August). *Aurasma / Chem* [Video file]. Retrieved from media.ggc.edu/media/t/1_u83n4h8a
2. Hoffman, M., & Provance, J. (2017). Visualization of molecular structures using HoloLens-based augmented reality. *AMIA Summits on Translational Science Proceedings*, *2017*, 68–74.
3. Tran, V., Lee, J., Kim, D., & Jeong, Y. (2016). Easy-to-use virtual brick manipulation techniques using hand gestures. *Journal Of Supercomputing*, *72*(7), 2752. doi:10.1007/s11227-015-1588-4
4. Noor, A. K. (2016). The HoloLens Revolution. *Mechanical Engineering*, *138*(10), 30-35.
5. Marvin, R. (2017). Microsoft's Mixed-Reality Plans Go Far Beyond HoloLens. *PC Magazine*, 111-116.
6. https://pubchem.ncbi.nlm.nih.gov/pug_rest/PUG_REST.html and https://pubchem.ncbi.nlm.nih.gov, retrieved on 10/1/2017. Last retrieved on 10/1/2017.

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