# Interactive AR Visualization of Molecular Simulation Data

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We present the software framework *chARp* — Chemistry Augmented Reality (AR) Package — and its first application, the *chARp* Molecular Builder [1], which is based on the virtual reality (VR) only prototype of Gebhardt et al. [2]. The overall aim is to bring immersive AR and VR techniques [3] to a chemistry-based application scenario. Currently, chARp runs as an AR application on the HoloLens2 and allows for live collaboration (see Figure 1) and hybrid workstation setups due to the freshly implemented networking extension that is based on Riptide [4]. The addition of the chemistry toolkit OpenBabel [5] provides several file I/O options and simplifies the pre-structuring of unstructured molecule data, such as the *xyz* file format. We are exploring the challenges and opportunities of an AR collaborative environment [6], specifically in this chemistry-based application scenario. Another project focus is to bring machine-learned (ML) models based on first-principles quantum-chemical calculations [7, 8] into the immersive environment to get immediate visual feedback and the possibility to interact with the ML model. Furthermore, we develop intuitive interactions and audio/haptic feedback and enhance the immersion with additional wearable devices [9].

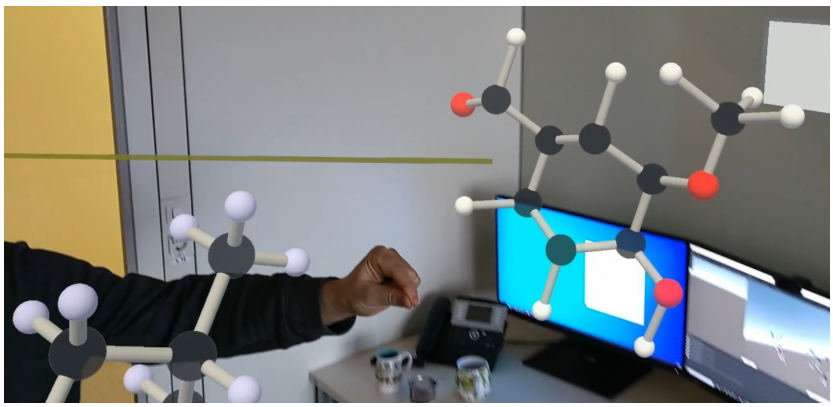

Figure 1: A grab of the View of the HoloLens2 while using the collaborative molecular building environment in chARp. In this case, two researchers are in the same virtual (and real) environment. The depicted view is from one person watching the other manipulating the ball-and-stick rendered molecules.

# References


[1] https://charpmolecularbuilder.github.io/ (last accessed: 2023-02-23)

[2] Gebhardt, Patrick and Yu, Xingyao and Köhn, Andreas and Sedlmair, Michael 2022. MolecuSense: Using Force-Feedback Gloves for Creating and Interacting with Ball-and-Stick Molecules in VR. *VINCI '22* ISBN: 978-1-4503-9806-0.

[3] Klein, K. and Sedlmair, M. and Schreiber, F. 2022. Immersive analytics: An overview. In *IT - Information Technology*, ISSN: 1611-2776

[4] https://github.com/RiptideNetworking/Riptide (last accessed: 2023-02-23)

[5] O'Boyle, Noel M. and Banck, Michael and James, Craig A. and Morley, Chris and Vandermeersch, Tim and Hutchison, Geoffrey R. 2011. Open Babel: An open chemical toolbox. *Journal of Cheminformatics* ISSN: 1758-2946.

[6] Sereno, Mickael and Wang, Xiyao and Besançon, Lonni and McGuffin, Michael J. and Isenberg, Tobias 2022. Collaborative Work in Augmented Reality: A Survey. *TVCG* ISSN: 1941-0506.

[7] Zaverkin, Viktor and Netz, Julia and Zills, Fabian and Köhn, Andreas and Kästner, Johannes 2022. Thermally Averaged Magnetic Anisotropy Tensors via Machine Learning Based on Gaussian Moments. In: *J. Chem. Theory Comput.* ISSN: 1549-9618.

[8] Zaverkin, Viktor and Holzmüller, David and Bonfirraro, Luca and Kästner, Johannes 2023. Transfer learning for chemically accurate interatomic neural network potentials. In: *Physical Chemistry Chemical Physics* DOI: 10.1039/D2CP05793J.

[9] Epstein, D.A., Blascheck, T., Carpendale, S., Dachselt, R. and Vermeulen, J. 2021. Challenges in Everyday Use of Mobile Visualizations. In Mobile Data Visualization. *Mobile Data Visualization.*