**Beyond Gaming: Virtual reality and real-time molecular dynamics for (bio)chemistry**

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Prior to widely available commodity computational machinery, room-sized models1 were popular within protein modelling and visualization in the 1950s/60s, allowing researchers to understand the first protein crystal structures. Models like these have played an important role in chemical research, allowing us to visualize the design intricacies of complicated nano-architectures across both biology and materials science. Driven by the consumer market, state-of-the-art virtual reality (VR) hardware now allows us to carry out broad new classes of video-gaming tasks which were previously impossible: wielding light-sabres, making 3d sculptures, and even simulating surgery. Applying these technologies to the molecular sciences allows us to re-engage with the sorts of large, immersive, tangible models that were once popular in molecular research.2, 3 Along with state-of-the-art advances in high performance computing (HPC), we can even go one step further: whereas the older models were time stationary objects that could only capture a single conformation of a molecule (e.g., a protein or DNA crystal structure), it is now possible to construct room-sized tangible and interactive models of molecular structures which are “animated” in real-time by rigorous dynamics, building on the significant progress made in computational molecular physics over the last 60 years.

In this presentation, I will discuss (and hopefully demo) the work we have carried out to design a new environment which fuses commodity VR and GPU-accelerated HPC to allow (up to 8) researchers to natively inhabit a fully interactive 3d virtual molecular simulation environment. Using wireless ‘atomic tweezers’, it is possible to fluidly chaperone a real-time research-grade biomolecular MD simulation in a fully co-located 3d space *with surgical precision*. This platform opens up a new domain of “interactive simulation”,4 allowing researchers to tackle a range of biomolecular design problems as they express their chemical design intuition to explore dynamical pathways and conformational states in hyperdimensional biomolecular systems. I will discuss some initial applications of our multi-person VR-HPC environment, including our attempts to understand the fundamental kinetic mechanisms and dynamical pathways whereby: (1) proteins form knotted structures, and (2) small molecular ligands (e.g., a drug or substrate) dock with a larger molecular receptor (a protein or enzyme).5

**[1]** Kendrew et al., Nature 181, 662 (1958);

**[2]** Glowacki et al., Multi Person Molecular Virtual Reality: <https://vimeo.com/200789130>;

**[3]** O'Connor et al., in *Supercomputing 2016* (2016);

**[4]** Glowacki et al., Faraday Discuss. 169, 63 (2014);

**[5]** Glowacki, O'Connor, Deeks, Interactive drug docking using real-time MD within the Nano Simbox: <https://vimeo.com/202556275>;