

Perceptualizing our Molecular World

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The ability to explore and understand the invisible world of molecules has evolved over millennia from philosophical conjecture to highly effective representational depictions and ever more capable interactive environments. Carroll Johnson was a pioneer in adapting computer technology to this effort. Using early computer driven pen plotters his ORTEP code enhanced the representation of molecular structure by using ellipsoids to depict the thermal motion captured in accurate x-ray crystallographic structures. It also made it possible for these structures to leap from the printed page by producing stereoscopic pairs, and became the standard for crystallographic structure publication.

To put this work in context, this talk will trace the advances of computational molecular graphics from the pen plotter to today's multi-modal visualization environments, and from the representation of simple organic molecules to that of molecular cellular environments. It will present a personal view of how technology and science have co-evolved to produce new representations and perceptual experiences that can go beyond the visual to enhance our understanding and abilities to interact with and explore the invisible molecular world. The advent of 3D printing, graphics processing units, game engines and virtual and augmented reality have created a new world in which we can advance our science and communicate it to the broader community.

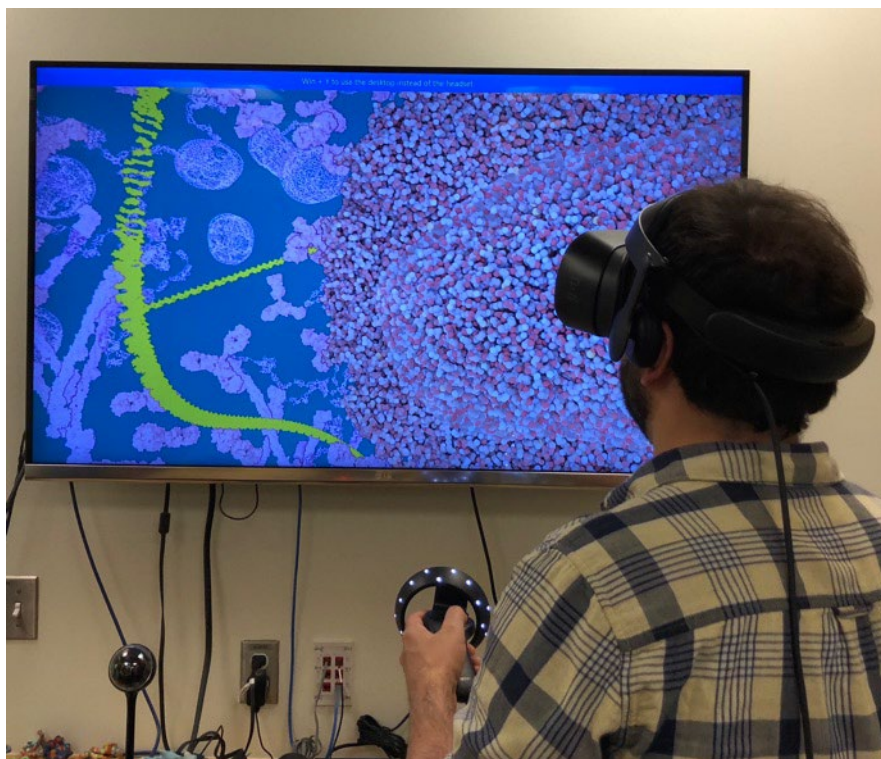


Figure 1