

## **Discovery through the lens of the computational microscope.**

The essential conundrum of modern biology, namely the question of how life emerges from myriad molecules whose behavior is governed by physical law alone, is embodied within a single cell—the quantum of life. The rise of scientific supercomputing has allowed for the study of the living cell in unparalleled detail, from the scale of the atom to a whole organism and at all levels in between. In particular, the past three decades have witnessed the evolution of molecular dynamics (MD) simulations as a “computational microscope”, which has provided a unique framework for the study of the phenomena of cell biology in atomic (or near-atomic) detail. Here I present an overview of our efforts to determine the molecular details during the life-cycle of multiple infectious diseases using the computational microscope .

### **Biography**

During my PhD, I was trained in computational biophysics by Prof. Tom Woolf at the Johns Hopkins University School of Medicine, developing theoretical and computational methods to discover molecular mechanisms governing the transitions between known protein stable states. During my postdoctoral training at the University of Illinois, under the leadership of the late Prof. Klaus Schulten, I developed and applied hybrid computational and experimental methods to determine the structure and chemical-physical properties of complete HIV and the Rous sarcoma virus capsids. This work revealed the need to develop small molecule anti-viral therapeutics with complete virus assemblies in mind, unlike the common practice of studying isolated virus components. During the past two years as an assistant professor, my group has co-authored 13 manuscripts on important human pathogens like HIV, HTLV and Chlamydia. My research is performed in close collaboration with a broad range of experimentalists including bacteriologists, virologists, immunologists, electron microscopists, X-ray crystallographers and NMR spectroscopists which allows our data-informed models to be validated.