



## Multiscale simulations of HIV replication

**Alvin Yu, Ph.D.**

Assistant Professor, Department of Physiology and Biophysics  
University of California, Irvine

**Abstract:** Physical simulations at the atomic level remain the most accurate method for describing biological complexes and macromolecular behavior. However, a central challenge persists in scaling both system size and timescale to capture phenomena that are biologically meaningful and medically relevant. In this talk, I will discuss our advances in understanding HIV biology using multiscale simulations to model viral particle maturation. Enhanced sampling strategies are utilized to reveal the energetics and mechanisms of conformational changes in capsid proteins, enabling the design of new maturation inhibitors. Furthermore, the development of “bottom-up” coarse-graining approaches provides high-fidelity mechanistic insights into capsid protein self-assembly. Finally, coarse-grained models of the complete HIV particle pave the way for simulations of micrometer-scale biological processes.

**Bio:** Alvin Yu is an Assistant Professor in the Department of Physiology and Biophysics. As a Ruth L. Kirschstein postdoctoral fellow in the Dept. of Chemistry at the University of Chicago, he studied the molecular basis for replication in viruses, including HIV and SARS-CoV-2. In his Ph.D. at Johns Hopkins University, he studied the physical and chemical basis for neural activity in glutamate receptor ion channels. He earned his B.S. in Physics from Caltech. He is a recipient of the K99/R00 grant from the National Institutes of Health. His research interests include developing and applying multiscale simulations to provide physical insight into living systems. He uses theory and computation to understand biological phenomena that have a direct impact on human health.

**Hosted by:** *Elizabeth Read*