UNIVERSITY OF DELAWARE

CHEMICAL & BIOMOLECULAR ENGINEERING

SPRING 2024 SEMINAR SERIES

MAKING THE INVISIBLE VISIBLE WITH THE COMPUTATIONAL MICROSCOPE

FEB 9 | 10:00 AM | 106 CENTER FOR COMPOSITE MATERIALS (CCM)

JUAN PERILLA

UNIVERSITY OF DELAWARE

Associate Professor

Attend virtually: https://udel.zoom.us/j/91386404306

The essential conundrum of modern biology, namely the question of how life emerges from myriad molecules whose behavior is governed by physical laws alone, is embodied within a single cell—the quantum of life. The rise of scientific supercomputing has enabled the study of the living cell in unparalleled detail, spanning from the scale of the atom to a whole organism and at all levels in between. As a result, the past three decades have witnessed the evolution of molecular dynamics (MD) simulations as a "computational microscope," providing a unique framework for the study of the phenomena of cell biology in atomic (or near-atomic) detail. The work in my group synergistically combines single-molecule biophysics, structural biology, and computational biology techniques to probe the molecular origin of biological phenomena. Here, I present an overview of our recent efforts to determine the molecular details during the life-cycle of a human pathogen: HIV-1. Our research uncovers intricate connections among the physical properties of the virus during two key infection events, namely cytoplasmic trafficking and nuclear entry. We validate our discoveries through in vivo infectivity assays on multiple cell lines to confirm their biological relevance. Altogether, the results from our work unveil the roles of essential cellular machinery in the virus life cycle, paving the way for the design of novel therapeutics. Lastly, I discuss the adaptability of our integrative computational-experimental methods to decode the molecular mechanisms of tumor viruses.

ABOUT THE SPEAKER

Dr. Perilla serves as an Associate Professor in the Department of Chemistry & Biochemistry at the University of Delaware. He earned his Ph.D. in 2011 from Johns Hopkins University, where his research focused on applying transition state theory to significant conformational changes in proteins. Following this, he joined the University of Illinois at Urbana-Champaign to conduct in silico studies of entire viruses under physiological conditions. His work emphasizes developing physical and chemical methodologies to comprehend biological processes associated with life and disease. His research encompasses a range from quantum-mechanical calculations to mesoscale simulations, utilizing the computational capabilities of petascale (and upcoming exascale) supercomputers. Prof. Perilla's team has also pioneered comprehensive molecular simulations of viral components, contributing to the advancement of a robust statistical analysis framework. He has published over 50 peer-reviewed papers, appeared on 11 journal covers, and contributed to three book chapters. Outside of academia, Dr. Perilla is an enthusiast of sports such as squash, and bike touring.

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