Physics
AT QUEENS COLLEGE

Colloquium Notice

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Building a computational microscope to investigate the design principles and functions of biomolecular machines

The health of our body is manifested at the cellular level by interactions between biomolecular machines. A mechanistic understanding of cellular processes at the molecular level is crucial for designing effective strategies to combat various diseases. In this seminar, I will present my work on developing a “computational microscope” that combines physics, molecular simulations, and machine learning to investigate exemplary molecular motor systems that play key roles in genome maintenance and cardiac muscle contraction. Firstly, I have developed rare-event sampling techniques based on statistical physics to search for the most probable transition pathways for biomolecular processes. The methodology enables me to capture the millisecond dynamics of helicase motors translocating nucleic acid substrates. Secondly, by integrating informatics approaches with molecular simulations, I was able to reveal how the myosin-actin complex generates force in the human heart muscle, providing insights into the allosteric network encoded in the machine. The computational platform directly links the protein sequence space to their functions. Finally, I will discuss my plans to study the emergent behaviors of the actin-myosin systems, engineer molecular motors with novel functions, and develop strategies for treating cardiomyopathy.

Wednesday
March 15, 2023
Starts at 12:15 PM
Coffee at 12:00 PM
Physics Conference Room, SB B326
This talk is accessible via **Zoom** or use
meeting ID 829 2687 2594 and **passcode 866995** to join