|  |  |
| --- | --- |
|  | Dr. Jun Fan, Assistant Professor Department of Physics and Materials Science City University of Hong Kong  Ph. D., Princeton University, Princeton, USA M. Sc., McMaster University, Hamilton, Canada B. Eng., Tsinghua University, Beijing, China   * Theoretical and Computational Materials Science and Biophysics * Assembly Molecular Self-assembly * Structure, Function and Dynamics of Cell Membranes and Proteins * Molecular Dynamics Simulations * Phase Field Modeling * Free Energy Calculations |

**From Materials Science to Biophysics – Continuum Modeling of Phase Transitions on Cell Membranes & Molecular Dynamics Simulations of Actin Filaments Mechanics**

The central role of materials science that the microstructure of a material links its formation processes and its properties applies to the fascinating biological systems. In this talk, I will present two examples to demonstrate it: formation and structure of cell membranes, as well as, the structure and mechanical properties of actin filaments.  The microstructure of cell membrane features lipid rafts, the liquid-ordered dynamic nanodomains, embedded in liquid-disordered matrices. Lipid rafts play an important role in transmembrane signal transduction, membrane trafficking, and viral budding. However, how the cell regulates the size, lifetime, and spatial localization of lipid rafts is still unclear. Over the years, experimental studies of lipid raft have lead to several phenomenological theories accounting for its formation. I investigated these theories by the continuum model and found that they can be differentiated by a combination of the spatial correlation and temporal fluctuation spectra of rafts. This result points the direction for the designing of experiments that will eventually lead to the correct paradigm of how cell regulates the microstructure of cell membranes.  The second example is about a protein system named actin. Actins assemble into actin filaments, which form mesh-like structure to support cell membrane.  The actin regulatory protein cofilin plays a central role in filament treadmill dynamics by severing filaments and increasing the concentration of ends from which subunits add and dissociate. Cofilin binding modifies the average structure and mechanical properties of actin filaments, thereby promoting fragmentation of partially decorated filaments at boundaries of bare and cofilin-decorated segments. Despite extensive evidence for cofilin-dependent changes in filament structure and mechanics, it is unclear how the two processes are linked at the molecular level.  Here, I use molecular dynamics (MD) simulations and coarse-grained (CG) analyses to evaluate the molecular origins of the changes in filament compliance due to cofilin binding.   This result displays the microstructure of actin filaments modified by cofilin affects the mechanical properties of filament.

工綜238, 10:00 am, 8月20日（星期二）