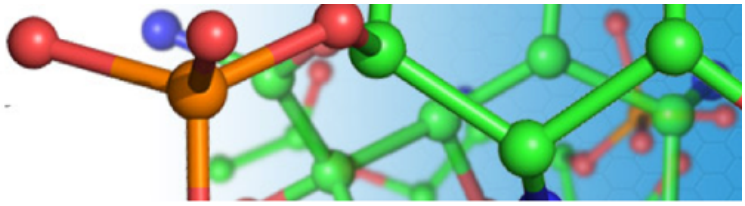
DEPARTMENT OF CHEMISTRY & CHEMICAL BIOLOGY

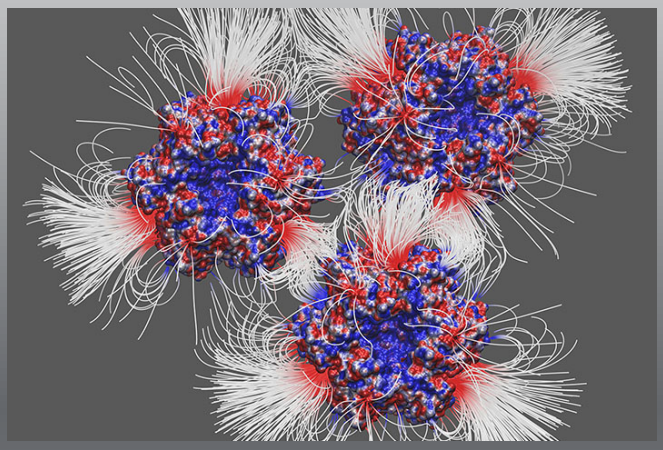


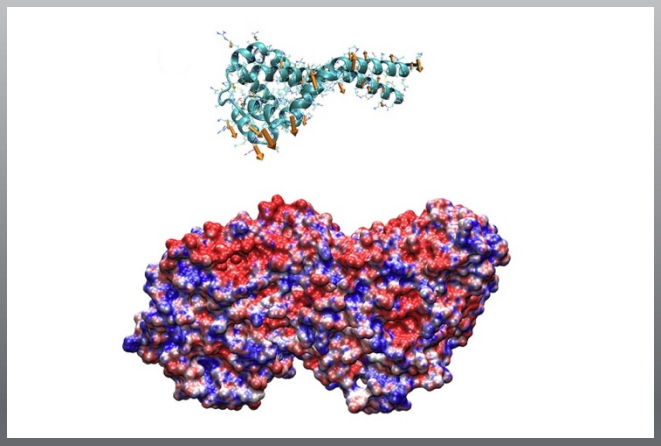
DEPARTMENT OF CHEMISTRY AND CHEMICAL BIOLOGY COLLOQUIUM

Presented by Lin Li, University of Texas, El Paso

Friday, March 22nd, 2019, at 4:00pm in the Science and Math Learning Center, Room 102

Reveal Mechanisms of Molecular Motors' Motilities and Viral Capsids Assembly Using Multi-Scale Approach





Protein-protein interactions play crucial roles in many biology phenomena. Therefore, a lot of efforts have been made to model the protein-protein interactions in biological systems. However, it is extremely challenging to accurately calculate the electrostatic interactions in large biological systems such as dynein and viral capsid. Dynein, a molecular motor, is important for cargo transportation and force generation in cells. Dysfunction of dynein is associated with many diseases, such as ciliopathies, lissencephaly and other neurodegeneration disorders. I will introduce a novel multi-scale simulation approach which was used to study dynein's motion along microtubules. The results demonstrate that the electrostatic interactions play significant roles in dynein's motilities and functions along microtubule. Understanding the fundamental mechanisms in molecular motors sheds light on curing many molecular motor related diseases. Besides molecular motors, viral capsid assembly was also studied by this multi-scale approach. Assembled by capsomers periodically, the viral capsid holds, protects and ejects the genes of the virus. Paramecium bursaria Chlorella virus (PBCV) was studied to study the capsid assembly mechanisms. Three different capsomer-capsomer binding modes were found in PBCV viral capsid, which reveals interesting and fundamental mechanisms for viral capsids assembly.