Physics & Astronomy Colloquium – Spring 2019

Tuesday, April 09th at 3:30 pm in SC 234

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Molecular Biophysics – From Protein Folding to Drug Design

Several state-of-art force fields for molecular modeling of biophysical systems in fact spin off from the molecular simulation of liquids. Since the first simulation of bovine pancreatic trypsin inhibitor (BPTI) in 1970s, bio-molecular simulations has come a long way now to capture cellular events at much longer time scale. Visualization of protein dynamics aided by high-resolution graphics with cutting edge software and hardware has strong experimental supportive correlation by NMR, Fluorescence and EPR spectroscopic techniques. In fact today's biophysics is a strong synthesis of several state-of-are research areas that include dynamic equations derived from Newtonian and Non-Newtonian mechanics, sophisticated applications of equilibrium and non-equilibrium statistical mechanics, high performance supercomputing resources, high energy synchrotron light sources for bio-macromolecular structure identification and so on. In my talk I will give a historical sketch of this fascinating developments of experimental and computational biophysics over several decades.

Also this scientific endeavors in 1990s attracted pharmaceutical industries to develop force field of organic molecules for bio-medicine applications that eventually made the field an essential stage in drug design with the outcome of developing physics-based large scale molecular docking programs to screen large chemical libraries. Optimizing and tuning ligands with protein structure based knowledge find enormous applications in modulation of protein properties and controlling its cellular signaling pathways for useful biological applications; a field popularly known as Computer Based Drug Design that in fact highly overlaps computational biophysics and chemistry and will be outlined for interested students. Finally I will present my recent molecular dynamics simulation results on two different G-protein Coupled Receptor (GPCR) systems, a variant of membrane protein popularly known to be the target of 50% of currently marketed drugs. And of course GPCRs will remain potential targets for many future bio-medicine applications and thus an area of active research for biophysics communities.

Refreshments at 3:00 pm in SC 103