Wednesday, October 20, 2021
4:00 P.M.

Ackert Hall, Room 120

Biochemistry & Molecular Biophysics **Seminar**

Peptide Design through Molecular Dynamics Simulation

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Peptides have emerged as a flexible, inexpensive, and biocompatible medium for designing functional molecules. This design is facilitated by molecular modeling, which has become increasingly reliable owing to improved methods and faster computers. In this talk, I will describe work in my group using computational tools to design peptides for applications from COVID-19 treatment to self-assembling nanostructures. We employ a multi-resolution approach beginning with sequence optimization and flexible docking using the Rosetta package, followed by screening of the free energy by the approximate MM-GBSA method. For a few of the most promising cases, we then apply rigorous free-energy calculations in explicit-solvent molecular dynamics simulation. Finally, we subject the peptides with the best predicted properties to experimental evaluation. We have experimentally verified the binding of a specially designed peptide to the SARS-CoV-2 spike protein and have observed the folding and self-assembly of another peptide at the graphite–water interface using AFM.