Protein Simulations in Confined Environments - M. Demirel (Pennslyvania State University)

Materials surfaces mimic cell like architecture and proteins can be encapsulated by these material surfaces. Depending on the number and types of surface interactions, this confine environment could destroy the protein or help it maintain its bioactivity. We are developing computer models and simulation tools for the understanding of surface-protein interaction at the atomistic levels. At the molecular level, molecular dynamics simulations are very powerful, but the high computational cost of molecular simulations is a drawback. A viable alternative method to study protein-receptor binding is the coarse-grained molecular simulations of simplified models, such as elastic network models. At the atomic interaction level, we use ab initio simulations to calculate the potential between surface and protein atoms.