

~~Special Polymer Physics Seminar ~~

Dr. Tao Wei

Materials Research Science and Engineering Center
& Department of Biomedical Engineering
Northwestern University

**10:00 AM Tuesday,
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301 Steidle Bldg.**

Modeling of Protein Adsorptions

Protein adsorption is a result of several competition processes: protein-surface interactions, protein hydration, surface hydration, and water-water interactions. Large-scale molecular dynamics simulation is used to study lysozyme orientation-dependent adsorption behavior on hydrophobic surfaces. Adsorption can be divided into three processes: diffusion to the surface, dehydration induced by hydrophobic surface-protein interactions, and denaturation. Protein's dehydration affects adsorption kinetics and can serve as a rate limit step. Dehydration on hydrophobic surface also disturbs protein domain's structural stability. The adsorbed protein can still display large and asymmetrical mobility on the heterogeneous surface. An understanding of protein adsorption mechanism at the atomistic scale is important for development of coarse-grained models and experimental surface design.