West Virginia University

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DEPARTMENT OF CHEMISTRY

Biomolecules at the Water-Nanomaterial Interface: An Atomic-Scale Perspective

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The combination of biomolecules and synthetic nanomaterials has exciting applications in biosensing, nanomedicine, and catalysis. However, design of materials for these applications requires insight into the atomic-scale interactions between relevant biological and synthetic components in an aqueous medium. Molecular simulation is a powerful tool for obtaining this insight, provided reliable computational models. In this talk, I will describe my group's efforts to validate and improve classical (force-field based) molecular dynamics models for describing interactions between organic molecules and synthetic nanomaterials in explicit aqueous solvent, leveraging enhanced sampling algorithms, analytical chemistry, and quantum mechanical calculations. Furthermore, I will show what molecular dynamics simulation can reveal about the adsorption thermodynamics and conformational equilibria of peptides and proteins on graphitic nanomaterials, including graphene, carbon nanotubes, and graphene oxide.

Date: Wed, Oct. 17, 2018
Time: 4:30-5:30 pm
Location: 208 Clark Hall

Students, meet the speaker over coffee and cookies in the Bennett Conference room at 3:30 pm