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SEMINAR

Molecularly Designed Interfaces for Biomaterials and Catalysts: Force-Field Based Simulation and New Theory

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Thursday, April 7, 2011
3:30 p.m., Chemistry Building 106

Refreshments will be served in Room 106

We will illustrate self-assembly mechanisms of biomolecules and inorganic nanostructures at the molecular scale by classical molecular dynamics simulation and experiment, and explain the development of force fields for the simulation biological-inorganic interfaces such as artificial bone materials and dental ceramics. Key aspects of the models are the assignment of atomic charges and van-der-Waals parameters which we have brought into quantitative consistency with surface and interfacial energies for the first time, as shown for the examples of various silicates and fcc metals. The adsorption of peptides in aqueous solution onto metal surfaces is controlled by coordination to epitaxial sites, and the influence of amino acid sequence and structure of the metal surface onto adsorption and crystal growth can be quantified by simulation in promising agreement with experiment. On silica surfaces, the adsorption of peptides is controlled by ion-pairing and a conformation-dependent pattern of hydrogen bonds. MD simulation using our models enables to understand the influence of single amino acid mutations in a peptide sequence upon adsorption to silica surfaces in aqueous solution in quantitative precision compared to adsorption measurements, and we discuss a range of surface models of silica with the equilibrium fraction of siloxide vs silanol groups as a function of pH and nanoparticle size.

We will also illustrate the use of complimentary quantum-mechanical simulations to elucidate electronic structure contributions and Monte Carlo simulation using customized coarse-grain models to explore the assembly of multiple peptides on surfaces. These and further computational examples that will be briefly mentioned include a range of collaborative efforts with experimental groups aiming at protein/inorganic complexes for biosensors and cancer therapeutics, polymeric additives for construction materials, tuning filler dispersion in nanocomposites, block copolymer assembly on templated substrates for nanoscale circuitry, understanding phase behavior of polyelectrolytes, and mineralization processes for artificial bone and dental materials. The connection of the models and simulation to the interpretation of structural and dynamic experimental data (X-Ray, imaging, spectroscopy, kinetics of self-assembly, adsorption) will be emphasized to explain guidance in synthesis and assembly of materials.