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Special Guest Lectures

Recent Progress in Development and Application of Non-Additive Interaction Models for Molecular Simulations of Biophysical and Physicochemical Systems**Sandeep Patel, University of Delaware**Johnston Hall 218
November 18, 2010 - 03:30 pm**Abstract:**

Molecular simulations today are applied across many scientific disciplines. Complementing experiment, these tools afford a molecular-level understanding and interpretation of physico-chemical processes at resolutions and timescales difficult or practically inaccessible to experiment. At the heart of such methods is the description of interactions between atoms and molecules, the force field. Traditionally, non-reactive force fields have treated electrostatic interactions using an additive, Coulomb model between fixed partial charges on atomic sites. Though quite successful, there has been conjecture as to the effects of incorporating non-additivity in classical force fields, particularly in biological systems. Over the last several decades, attempts to incorporate electrostatic non-additivity in the form of inducible dipole interactions or dynamically varying partial charges have provided a vast body of knowledge that has aided in the development of a new class of force fields attempting to explicitly account for non-additive effects. We will present our recent work in developing one such class of models, charge equilibration force fields, and applications of such models to aqueous solution interfaces, model membrane bilayers and simple integral membrane peptides such as the gramicidin A bacterial channel, and recent work on modeling of protein-ligand interaction free energetics. Access Grid viewing is in 218 Johnston Hall. Live presentation is at the University of New Orleans.

