

Multiscale Modelling of Screening and Crowding in Soft Materials

Prof. Alan Denton
Physics Department
North Dakota State University
Fargo, ND, USA

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ABSTRACT: Soft matter systems -- multicomponent mixtures of giant and small molecules -- have attracted much attention recently for their rich physical properties and promise for engineering novel materials. For example, colloidal crystals are widely explored for photovoltaic and photonic applications, with practical importance for solar cells, optical switches, and (potentially) quantum computers. In colloidal suspensions and polyelectrolyte solutions, microion screening of electrostatic forces between macroions influences the structure and stability of many common materials, from foods to pharmaceuticals. Electrostatic screening can be modified by the addition of nanoparticles, enriching the tunability of interparticle forces and phase stability. In polymer-nanoparticle mixtures, crowding by hard particles can induce demixing and modify conformations of soft polymer coils, with biological relevance for protein and RNA folding. In modelling such complex systems, multiscale approaches help surmount computational challenges posed by diverse length and time scales and provide physical insight into experimental observations. In this talk, I will outline our recent efforts to model screening and crowding effects and to explore by molecular simulation the stability and structural properties of soft materials.

ALL ARE WELCOME!!!