Physical Chemistry Seminar

Tuesday, February 17, 2015 | **11:00 am** | **Room 1315 Chemistry Building**

Coarse grained models for macromolecules

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Macromolecular systems have interesting behavior on a range of length-scales and timescales. Computational study of these systems therefore requires modeling at multiple levels of detail. The development of coarse-grained (CG) models for macromolecules is an exciting and challenging frontier of research in computational chemistry. The ultimate goal is to develop a model that is computationally feasibly but captures the essential physical chemistry. We have developed a CG model of water called the big multipole water (BMW) model where four water molecules are grouped into one site. I will discuss the performance of this force field for several problems including the hydrophobic effect, the behavior of peptides at membranes, the self-assembly and phase behavior of lipid/peptide mixtures, and the conformational properties of polymers. The results highlight the utility of coarse-grained models as well as some pitfalls when applied to polymer solutions.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315