Abstract:
Coarse grained force fields for molecular liquids and polymers frequently represent the intermolecular interactions with effective potentials that cannot easily be physically interpreted. This unsatisfactory fact limits our understanding of the model's representability (which physical properties other than the ones used in the parameterization can or cannot be described?) and transferability (can the model be used at different densities, temperatures, ionic strengths, etc.?). I will present some of our recent work in which effective potentials have been obtained through computation of the conditional reversible work (CRW) expended upon introducing nonbonded interactions between atom-groups or between entire molecules. Examples shown in my talk include polymers, molecular liquids, and small molecules in aqueous solution. The representability and transferability of the CRW-potentials will be discussed.