Lecture 3: New Challenges for Modeling Chemistry in Solution
9:45 a.m. Thursday, November 8, 331 Smith Hall

The correct representation of intermolecular interactions using force fields is essential to their utility in simulations of organic and biomolecular systems as well as new materials. Two issues that have been addressed recently are halogen bonding and the interaction of water and ions with extended π-systems including acenes, graphene, and nanotubes. For halogen bonding, the classical point charge model requires augmentation with a partial positive charge on the C-X axis to represent the σ-hole for aryl chlorides, bromides, and iodides. The enhanced force fields, OPLS-AAx and OPLS/CM1Ax, have been tested in calculations on gas-phase complexes and for free energies of hydration, densities, and heats of vaporization of halobenzenes. For the extended π-systems, the OPLS-AA force field is found to perform very well in comparison to CCSD(T)-level calculations for complexes with a water molecule. However, proper representation of interactions with ions requires addition of polarization such as with inducible dipoles in the OPLS-AAP force field.