Abstract for an Invited Paper
for the MAR07 Meeting of
The American Physical Society

Local and global refinement of electronic and structural properties of proteins via QM/MM

JOSE GASCON, University of Connecticut

This talk presents a new method to incorporate polarization effects in the electrostatic potential of proteins and enzymes, with potential application to even larger biological systems such as ribosomes. Polarization effects are incorporated via an iterative self-consistent point-charge model of the protein electrostatic potential. The method, which scales linearly with the size of the protein, achieves quantitative agreement with full QM calculations in the description of electrostatic potentials of small polypeptides where polarization effects are significant, showing a remarkable improvement relative to the corresponding electrostatic potentials obtained with popular MM force fields. The capabilities of the method will be demonstrated in several applications, including calculations of the electrostatic potential in the potassium channel protein and the description of protein-protein association.