Charge view of the Poisson-Boltzmann equation

Xiang Ye and Ray Luo

Department of Molecular Biology and Biochemistry, University of California, Irvine, CA 92697

We present a rigorous formulation of electrostatic energy and force with polarization charges. We first show that electrostatic potential can be viewed as summation of coulombic potentials due to atom charges and reaction field potentials due to polarization charges. Following this decomposition the energy and forces (both reaction filed and dielectric forces) can be recast into a form using polarization charges. This charge view method, which replaces the solvation effect with surface polarization charge effect, can avoid the numerical discontinued singularity at dielectric interface. And a series of numerical tests show that the calculated energy and forces are converged better than standard finite-difference method.