

# Charge view of the Poisson-Boltzmann equation

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We present a new rigorous formulation of energy and force on Poisson-Boltzmann equation (PBE). Electrostatic effects are computed by first calculating the distribution of polarization charge located on the molecular surface. The reaction field force on a particular atom is then calculated by summation the coulombic interaction with the induced surface charge. This charge view method, which replaces the salvation effect with surface polarization charge effect, can avoid treating the discontinuity of the dielectric. And a series of numerical tests show that the calculated energy and forces by this method agree well with the finite-difference approximation.