Modifying Poisson Equation for Near-Solute Dielectric Polarization

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The dielectric polarization $\boldsymbol{P}$ is significant for calculating the solvation free energy of biomolecules and the electromagnetic interactions between charged atoms in dielectrics. $\boldsymbol{P}$ was decomposed into the product of the electric dipole moment per molecule, $-\boldsymbol{p}$; the bulk solvent density; and the relative solvent molecular density, $-g$. For the molecular solute, $4\pi r^2\boldsymbol{p}(r)$ oscillates with the distance r to the solute, and $g(r)$ has a large peak in the near-solute region as observed in molecular dynamics (MD) simulations. Herein, the Poisson equation was modified for computing $\boldsymbol{p}$ based on the modified Gauss's law of Maxwell's equations, and the potential of mean force was used for computing g. For a one-particle solute in water, the $4\pi r^2\boldsymbol{P}(r)$ calculated from the derived equations behaves in an oscillatory manner with the distance to the solute r as shown by MD simulations.