

Continuous dielectric permittivity I: Specific features of the dielectric continuum solvation model with a position-dependent permittivity function

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We consider a modified formulation for the recently developed new approach in the continuum solvation theory (Basilevsky, M. V., Grigoriev, F. V., Nikitina, E. A., Leszczynski, J., J. Phys. Chem. B 2010, 114, 2457), which is based on the exact solution of the electrostatic Poisson equation with the space-dependent dielectric permittivity. Its present modification ensures the property $\text{curl } \mathbf{E} = 0$ for the electric strength field \mathbf{E} inherent to this solution, which is the obligatory condition imposed by Maxwell equations. The illustrative computation is made for the model system of the point dipole immersed in a spherical cavity of excluded volume.

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