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

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(Submitted on 2 Jul 2011 (v1), last revised 10 Aug 2011 (this version, v2))

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 curl E = 0 for the electric strength field 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.

Submission history

From: Oleg Kupervasser [view email]

[v1] Sat, 2 Jul 2011 19:38:02 GMT (317kb)

[v2] Wed, 10 Aug 2011 12:28:31 GMT (317kb)

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