

Abstract Submitted  
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**Rigorous treatment of electrostatics for spatially varying dielectrics: how far can one go using energy minimization?**<sup>1</sup> YI-KUO YU, OLEG OBOLENSKY, RAJARSHI RAY, T. DOERR, National Center for Biotechnology Information/NIH — A novel energy minimization formulation of electrostatics that allows computation of the electrostatic energy and forces to any desired accuracy in a system with arbitrary dielectric properties is presented. An integral equation for the scalar charge density is derived from an energy functional of the polarization vector field. This energy functional represents the true energy of the system even in non-equilibrium states. Arbitrary accuracy is achieved by solving the integral equation for the charge density via a series expansion in terms of the equation's kernel, which depends only on the geometry of the dielectrics. The streamlined formalism operates with volume charge distributions only, not resorting to introducing surface charges by hand. Therefore, it can be applied to arbitrary spatial variation of the dielectric susceptibility. The simplicity of application of the formalism to real problems is shown with three examples.

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