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Nonlinear functional for solvation in Density Functional Theory[1] DENIZ GUNCELER, RAVISHANKAR SUNDARARAMAN, KATHLEEN SCHWARZ, KENDRA LETCHWORTH-WEAVER, T. A. ARIAS, Cornell University — Density functional calculations of molecules and surfaces in a liquid can accelerate the development of many technologies ranging from solar energy harvesting to lithium batteries. Such studies require the development of robust functionals describing the liquid. Polarizable continuum models (PCM's) have been applied to some solvated systems; but they do not sufficiently capture solvation effects to describe highly polar systems like surfaces of ionic solids. In this work, we present a nonlinear fluid functional within the framework of Joint Density Functional Theory. The fluid is treated not as a linear dielectric, but as a distribution of dipoles that responds to the solute, which we describe starting from the exact free energy functional for point dipoles. We also show PCM's can be recovered as the linear limit of our functional. Our description is of similar computational cost to PCM's, and captures complex solvation effects like dielectric saturation without requiring new fit parameters. For polar and nonpolar molecules, it achieves millihartree level agreement with experimental solvation energies. Furthermore, our functional now makes it possible to investigate chemistry on the surface of lithium battery materials, which PCM's predict to be unstable.

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