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Universal continuum solvation models for plane-wave density functional theory DENIZ GUNCELER, T.A. ARIAS, Cornell Univ — Electron density based continuum solvation models have progressed rapidly over the last few years. This has enabled the application of electronic structure methods, especially density functional theory, to many problems at solid-liquid interfaces. One limitation of these iso-density methods is that they are often parametrized only for aqueous solutions and not for many other solvents used in technological applications (for example, organic solvents). To overcome this defficiency, we present an algorithm for constructing "universal" isodensity models by using readily available thermodynamic quantities of the solvent (such as dielectric constant and vapor pressure). We also disscuss the applications of the resulting model, implemented in the open-source plane-wave code JDFTx, to the stability of anode surfaces in Lithium batteries.

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