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A priori **classical density functionals of water: toward first principles exploration of aqueous based energy systems** RAVISHANKAR SUNDARARAMAN, KENDRA LETCHWORTH WEAVER, TOMAS ARIAS, Cornell University — The microscopic structure of inhomogeneous water plays a critical role in the properties of a wide variety of important energy systems including fuel cells and photoelectrochemical cells. Joint density functional theory has proven to be an efficient tool for the quantum-mechanical modeling of systems such as Pt electrodes in the presence of water, but requires theories for water which go beyond semi-empirical continuum solvation models, and accurate models for the coupling between water and electronic systems [1]. Toward this end, we present a new density-functional description of liquid water capable of predicting interatomic correlation functions, the linear and nonlinear dielectric response, and solvation energies without empirical fit parameters. The functional itself is built upon the site-potential representation of the ideal gas, a hard sphere reference fluid for the repulsive correlations, and an equation of state that reproduces the bulk properties of water over the entire extent of its liquid phase. Hydrogen bonding, the local tetrahedral structure and orientational correlations are captured *a priori* by a density-functional reformulation of the Kirkwood model for the dielectric constant.

[1]K. L. Weaver et al, to be presented at APS March Meeting 2011

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