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Surface Studies with Combined Free Energy Functionals of Electronic and Liquid Densities[1]

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— The microscopic structure of both a solid surface and a contacting liquid can be dramatically affected by the interaction between the two systems, particularly at the interface between a polar surface and a polar liquid. We present a study of oxide and metallic surfaces in an aqueous electrolyte environment with Joint Density Functional Theory (JDFT), a computationally efficient alternative to molecular dynamics simulations which replaces thermal sampling with a single variational principle for the free energy of the full system. Within the rigorous framework of JDFT, we introduce classical density-functionals for ionic species and describe how to couple them with existing functionals for liquid water and traditional electronic density-functionals. Calculations employ a liquid water functional, which captures bulk properties and microscopic structure over the entire phase diagram of the liquid, and a density-only coupling functional between the electronic and liquid systems, which can reproduce solvation free energies of small molecules to within chemical accuracy. With this microscopically accurate description of the liquid-solid interface structure, we gain physical insight which could direct future studies of catalysis and electrode stability in electrochemical systems.

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