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Self-consistent continuum solvation of electrodes in electrochemical environments STEPHEN WEITZNER, ALI KACHMAR, ISMAILA DABO, Department of Materials Science and Engineering, The Pennsylvania State University — Implicit solvent models have been widely used to study quantum systems in solutions. Nevertheless, these models differ considerably in their phenomenological details and in the complexity of their parameterization. While conventional implicit models rely on atomic positions and tabulated atomic radii to construct the solvation shell that surrounds the quantum solute, recent models aim to reduce the number of parameters by building solvation shells directly from the computed electronic densities. The self-consistent continuum solvation (SCCS) model, which belongs to this latter class, has been shown to reproduce the solvation energies of a wide range of molecular species in very satisfactory agreement with experiment, using only two fitted parameters [J. Chem. Phys. 136, 064102 (2012)]. Here, we report on the performance of the SCCS model in describing the electrical properties of quantum electrodes embedded in continuum electrolytes. We show that one additional parameter is necessary to capture experimental shifts in the neutral electrode potential as a function of surface composition and structure, and to correctly calibrate computed results to a common electrochemical reference. Directions for further improvement are also discussed.

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