

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Self-consistent continuum solvation (SCCS): Towards the accurate modeling of electrochemical systems in plane-wave DFT STEPHEN WEITZNER, ISMAILA DABO, The Pennsylvania State University — Implicit solvent models have been widely used to study quantum systems in solutions. Nevertheless, these models differ greatly 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 computed electronic densities. The self-consistent continuum solvation (SCCS) model, which belongs to the latter class, has been shown to reproduce the solvation energies of a wide range of molecular species in good agreement with experiment, using only two fitted parameters [J. Chem. Phys. 136, 064102 (2012)]. Here, we report on the SCCS model's performance in describing the electrical properties of quantum electrodes embedded in continuum electrolytes. We show that one additional parameter is needed 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. Utilizing this approach, we establish a novel framework for studying interfacial electrochemical phenomena.

Stephen Weitzner
The Pennsylvania State University

Date submitted: 14 Nov 2014

Electronic form version 1.4