Finite Bias Calculations to Model Interface Dipoles in Electrochemical Cells at the Atomic Scale - DTU Orbit (09/11/2017)

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The structure of an electrochemical interface is not determined by any external electrostatic field, but rather by external chemical potentials. This paper demonstrates that the electric double layer should be understood fundamentally as an internal electric field set up by the atomic structure to satisfy the thermodynamic constraints imposed by the environment. This is captured by the generalized computational hydrogen electrode model, which enables us to make efficient first-principles calculations of atomic scale properties of the electrochemical interface.

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