Cyclic Voltammmograms from First Principles - DTU Orbit (24/12/2018)

Cyclic Voltammmograms from First Principles

Cyclic voltammetry is a fundamental experimental tool for characterizing electrochemical surfaces. Whereas cyclic voltammetry is widely used within the field of electrochemistry, a way to quantitatively and directly relate the cyclic voltammogram to ab initio calculations has been lacking, even for the simple case of electroadsorption and desorption of H. In the following we derive the cyclic voltammogram for H adsorption and desorption on Pt(111) and Pt(100) based solely on density functional theory calculations and standard molecular tables. The method will also be extended to include the potential dependence of the OH coverage during electrochemical water splitting on Pt(111) and Pt3Ni(111).

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