Molecular level modelling of electrochemical reactions

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Abstract:
I will present an overview of density functional theory (DFT) based molecular modelling of hydrogen and oxygen evolution reactions (HER and OER). The emphasis is on the fast screening type modelling (ΔG) of various catalyst. We have studied HER on several different catalyst, including carbon nanotube (CNT) based materials [1], MoS_2 [2] and Ni_2P [3]. In addition, the OER can be studied with ΔG-type models [4]. In all these studies, the role of catalyst doping has been addressed. On MoS_2 and Ni_2P, the metal doping has been considered and in CNT the N doping has been studied in detailed [1,4]. Some remarks of the limitations of the ΔG model and models with explicit water molecules will be discussed. Overall, the molecular modelling of electrochemical reactions in under intense development and many new methods have been introduced recently. One of them is the use of contrained-DFT for studying coupled electron-proton transfer reaction [5].

Key words: Density Functional theory, hydrogen evolution reaction, oxygen evolution reaction, catalysis

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