An ab-initio Study of Hydrogen Atom Catalysis and Diffusion in Nickel Oxy/hydroxide

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Production of electric power by solar splitting of water and the reveres process in a fuel cell is a major source of renewable energy. One of the best known catalysts for water splitting is nickel hydroxide doped with iron. Although NiOOH is a widely researched material, the hydrogens position in it are not fully known. We used density functional theory + U (DFT+U) calculations to model hydrogen transfer under the surface during oxygen evolution reaction catalysis in pure and Fe doped NiOOH. Our calculations provide further evidence to the improvement of the catalysis by doping with Fe.[1]

Additionally, we carried out Nudged Elastic Band (NEB) calculations of hydrogen diffusion in the bulk of several related phases, including β-$Ni(OH)_2$, β-NiOOH and α-$Ni(OH)_2$. We considered vacancies and interstitial diffusion mechanisms and found the activation energy and minimum energy path for diffusion. Our results show that hydrogen diffusion is plausible in between the sheets of each phase. Furthermore, results suggests that as the material become charged (β-NiOOH, 50% hydrogens) the formation of interstitial hydrogens is spontaneous and the activation energy become as of the activation energy of vacancy in the discharged phase (β-$Ni(OH)_2$, 100% hydrogens). We conclude that hydrogen diffusion is more effective in the charged state.

1. Elbaz, Y. & Caspary Toroker, M. Dual Mechanisms: Hydrogen Transfer during Water Oxidation Catalysis of Pure and Fe-Doped Nickel Oxyhydroxide. *J. Phys. Chem. C* **121,** (2017).