The University of Texas at Austin
Energy Institute

The University of Texas at Austin
McKetta Department of Chemical Engineering
Cockrell School of Engineering

Computational Modeling of Nickel Oxyhydroxide For Water Splitting

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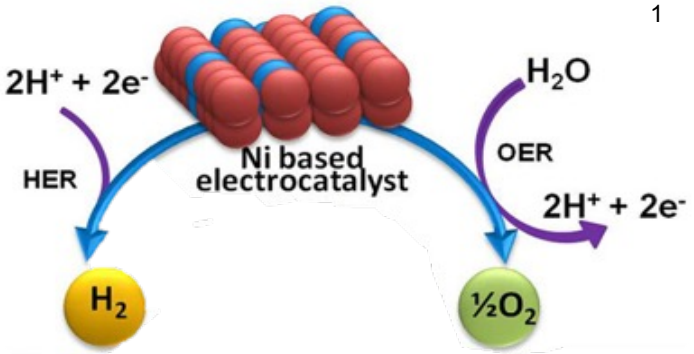
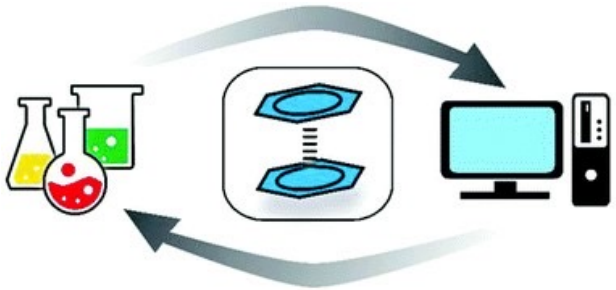
Jing Lian Ng, Kenta Kawashima, Yoon Jun, Joaquin Resasco, C. Buddie Mullin, Wennie Wang

Image from: https://news.mit.edu/2020/how-ruthenium-dioxide-splits-water-0521

Elucidating the Role of Structural Disorder in OER of (Oxy)hydroxide Electrocatalysts



[1]



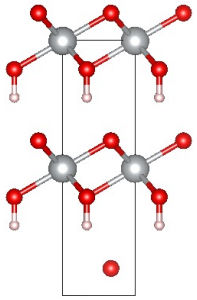
- Oxygen evolution reaction (OER) is the kinetically limiting step in electrochemical water splitting
- Nickel (oxy)hydroxide exhibit promising OER catalytic performance in alkaline media[2]
- Catalytic activity can be enhanced by:
  - Transition metal alloying
  - Introduction of structural disorder (amorphous structure)
- Optimization of $Ni_{1-x}Fe_xOOH$ is hindered due to poor knowledge on structure-activity relation

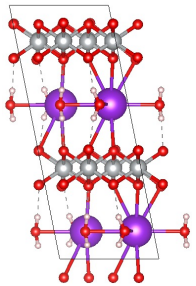
- Combined computational and experimental approach
- Benchmarking simulated and measured XAS to study structure-activity relationship
- Elucidate combined effect of mixed transition metal and amorphization on catalytic performance

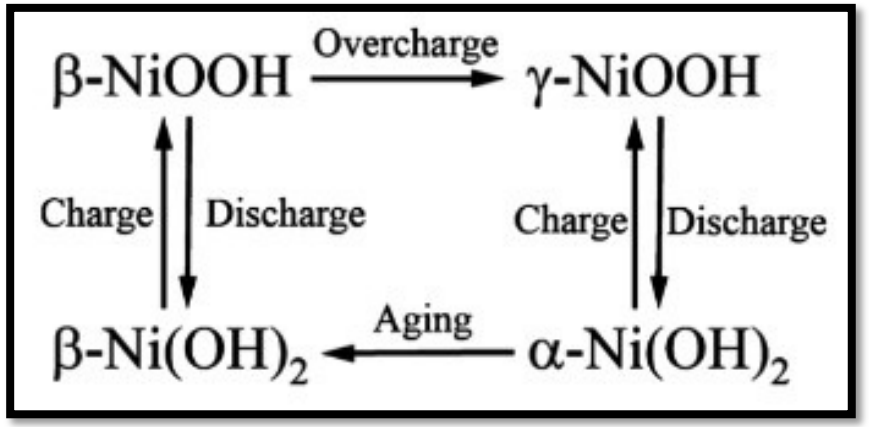
- Establishing baseline:
  - Determining the structure of nickel (oxy)hydroxide, NiOOH
  - Determine the level of theory to predict the structures using Density Functional Theory (DFT)

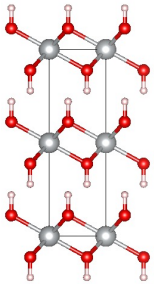
1. Figure adapted from: ACS Catal., 2017,7(10), 7196-225 doi:10.1021/acscatal.7b01800
2. J Phys. Chem. C., 2015,119(43), 24315-22 doi: 10.1021/acs.jpcc.5b08481

Structural Transformation of NiOOH



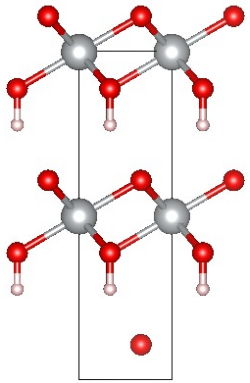




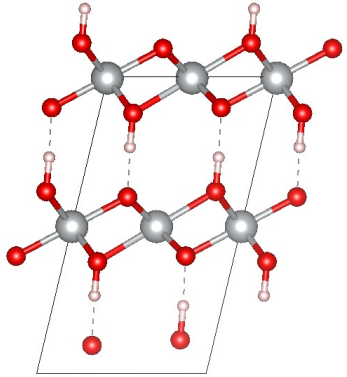


- Exact structure of NiOOH is not known due to poor resolution in XRD analysis
- All redox species of NiOOH consists of layers of NiO_2 with different hydrogen composition
- β- and γ-NiOOH similar in structure, where γ- phase consists of intercalated ions
- Synthesis of β-NiOOH requires an ion-free environment

DFT Evaluation of β-NiOOH Atomic Structure

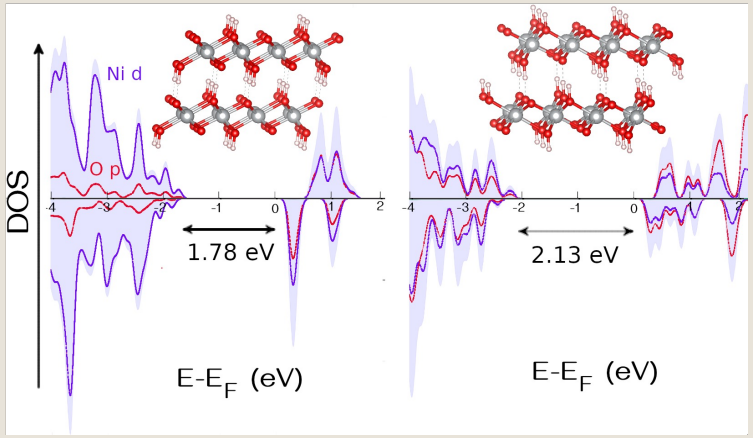


Native Structure

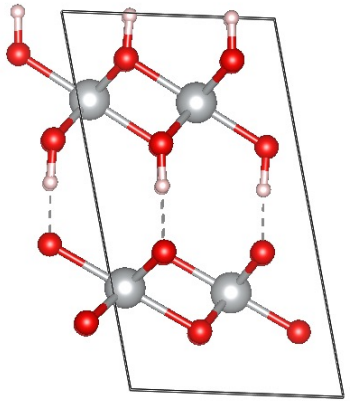


Staggered Structure

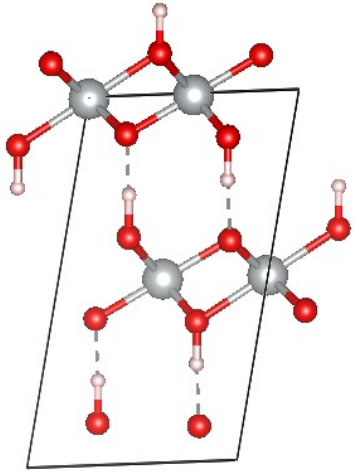
- Electronic structure of NiOOH is sensitive to hydrogen configuration



- Relative energy difference as low as **0.005 eV** between **alternate-layer** and **modified staggered** structure
- β-NiOOH bulk structure could consist of a mixture of alternate-layer and modified staggered structure



Alternate-Layer Structure



Modified Staggered Structure