

סמינר SEMINAR

Theoretical Characterization for Nickel Oxyhydroxide-One of the best Water Oxidation Catalysts for Energy Applications

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Solar energy conversion through water splitting in a photo-electrochemical cell is one of the most popular fields in recent years. Therefore, efficient anode and cathode materials at low cost are essential. An outstanding inexpensive catalyst that is considered to be one of the best for Oxygen Evolution Reaction (OER) is nickel oxyhydroxide (NiOOH). This reaction at the anode is especially challenging as there are very few materials that are able to perform the catalysis efficiently.

A promising material for catalysis should have appropriate band edge positions. Unfortunately, no study has analyzed the electronic band edge positions of NiOOH, which is a critical characteristic for catalysis feasibility.

In this seminar, I will present first-principles calculations of band edge positions for surfaces of pure NiOOH. Specifically, the band edge positions of NiOOH (001), (100), and (01 $\bar{5}$) were calculated using density functional theory (DFT) methods by using slab models.

Besides the band edge positions, I will briefly present more results that contributes to understanding the nature of NiOOH's success. It includes the effect of hydrogen vacancies and Fe doping on NiOOH ability to catalyze OER, and electronic structure of bulk NiOOH with hydrogen vacancies.

Supervisor: Prof. Maytal Caspary Toroker

ההרצאה תתקיים ביום ראשון, ה-8 בינואר 2017 בשעה 14:30
באודיטוריום ע"ש דיוויד וואנג, קומה 3, בנין דליה מידן

**The lecture will take place on Sunday, January 8th, 2017 at 14:30
David Wang Auditorium, 3rd floor, Dalia Maydan Bldg.**

כיבוד קל יוגש לאחר הסמינר