



## **Wolfson Department of Chemical Engineering Seminar**

**Lecture Hall 6, Wolfson Department of Chemical Engineering,**

**Wednesday April 5 2017 at 13:30**

# **Dr. Jeremie Zaffran**

## **Technion**

### **Computational design of solid catalysts: An application of the Density Functional Theory (DFT)**

During the last decades the Density Functional Theory (DFT) has attested of its high interest in the computational design of solid catalysts. We will present here two examples to illustrate how DFT can be used to tune catalytic properties of materials in the area of clean energy. In the first one, we will focus on solar energy application and the elaboration of efficient anodes for water splitting in photoelectrochemical cells. In the second one, we will consider biomass conversion, and we will present a method for fast screening of the reactivity of such complex molecules.

First, we will discuss of solar water splitting. Oxygen Evolution Reaction (OER) is the major challenge of such technologies. That reaction occurs at the anode of photoelectrochemical cells and consists in water molecules oxidation towards oxygen gas. So far, nickel oxyhydroxide (NiOOH) is one of the best catalysts known for this task. However, NiOOH properties are strongly doping dependent. To this date, only Fe is known experimentally to be efficient to significantly improve surface activity of NiOOH. In this project, we used DFT based calculation in order to scan the potential interest of several other metallic elements. Considering the first d row of the periodic table transition metals (TM) block, we were able to show that late TM are generally preferable for OER process on NiOOH catalyst. We were able to correlate such observations to adsorption strength of some key reaction intermediates, and to the metal-oxygen bond ionicity in the bulk.

In the second topics, we will discuss of biomass reactivity. Biomass molecules are complex and highly time consuming when using first principles calculation methods. While reaction energy ( $\Delta E$ ) may be relatively easy to reach, activation barriers ( $E^\ddagger$ ) can require several days or week of calculation with DFT. To tackle this time issue, we built Brønsted-Evans-Polanyi (BEP) linear relationships. Such methods, allow a direct prediction of  $E^\ddagger$  from the DFT computed  $\Delta E$ . Starting from monoalcohol dehydrogenation on metallic surfaces, we developed BEP models. We showed that such relations could predict glycerol (taken as a model polyol) dehydrogenation on Rh with an average error of 0.10 eV. Finally we will explain on a test case how to use those methods to simplify a complex reaction network.

Refreshments will be served at 13:15