

The 219<sup>th</sup>

# MANA Seminar



## The thermochemistry of oxidative dehydrogenation of a water molecule at a TiO<sub>2</sub>/water interface

Chair: Dr. Yoshi Tateyama (MANA Scientist)



### Prof. Michiel Sprik

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The standard potential vs the normal hydrogen electrode for oxidative dehydrogenation (ODH) of H<sub>2</sub>O is 2.7V. One might hope that electrocatalysts for oxidation, such as transition metal oxides, can bring this energy down. We have investigated this question for a water molecule adsorbed on the rutile TiO<sub>2</sub> (111) surface using Density Functional Theory based Molecular Dynamics (DFTMD) methods. A first challenge in this computation is to check that the method can reproduce the ODH potential in bulk water. Exploiting the latest advances in the CP2K (cp2k.berlios.de), we find 2.5V, encouragingly close to the target value of 2.7V. Adsorption on the TiO<sub>2</sub>/water interface reduces the ODH potential to 2.0V. However, resolving the dehydrogenation in an acid dissociation and oxidation of the hydroxide anion, it appears that most of this the 0.5 eV activation by the surface is due to an increase in acidity. After outlining the DFTMD method, we will make an attempt in this talk to give an explanation for these observations. This work is in collaboration with Dr. Jun Cheng.

**Venue: 4F, Seminar room #431, MANA Bldg., Namiki Site**

**Date: September 9<sup>th</sup> (Fri) Time: 15:30-16:15**

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