הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע״ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar
Lecture Hall 6, Wolfson Department of Chemical Engineering,
Wednesday March 21st at 1:30pm

Prof. Maytal Caspary Toroker

Materials Science and Engineering Department – Technion

Advances in modeling water splitting with iron oxide

Iron(III) oxide (α-Fe2O3) is widely considered a promising material for converting solar energy through oxidizing water. In this talk, I will highlight several of our insights that result from modeling water oxidation with Fe2O3. We rule out the existence of a stable peroxo Fe–O–O–Fe adsorbate and show that the origin of a surface absorption peak could be a Fe–O· type bond that functions as an essential intermediate of water oxidation. In agreement with experiment, we find that α-Al2O3 coverage decreases the overpotential required for water oxidation on α-Fe2O3. We explain this improvement through the decrease in the work function of α-Fe2O3 upon α-Al2O3 coverage that aids in extracting electrons during the water oxidation reaction. We also model a nano-Fe2O3 sheet and conclude that Fe2O3 should be grown on a substrate with a similar lattice constant to reduce strain and improve catalytic efficiency. This research contributes to understanding the chemical nature and role of electrode electronic surface states, which is crucial for improved electrochemical cell operation.

References:

1. M. H. Dahan and M. Caspary Toroker, "Water oxidation catalysis with Fe2O3 constrained at the nanoscale", J. Phys. Chem. C, 121(11), 6120 (2017).
2. O. Neufeld, N. Yatom, and M. Caspary Toroker, "A first principles study on the role of an Al2O3 overlayer on Fe2O3 for water splitting", ACS Catalysis 5, 7237 (2015).
3. N. Yatom, O. Neufeld, and M. Caspary Toroker, "Toward settling the debate on the role of Fe2O3 surface states for water splitting", J. Phys. Chem. C 119 (44) 24789 (2015).

Refreshments will be served at 1:15pm