

סמינר SEMINAR

Solar Water Splitting with α -Fe₂O₃ based Photocatalysis: a Theoretical Approach

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Photoelectrochemical cells (PEC) offer a promising way to convert solar energy to hydrogen fuel through water splitting. A common photoanode used in these cells is iron(III) oxide, also known as hematite, or α -Fe₂O₃. This material has many advantages, but unfortunately suffers from poor conductivity, high electron-hole recombination rates, and a large overpotential required for water splitting. Several strategies for overcoming these issues and improving the PEC efficiency have already been put forward. However, more progress is still needed, and this requires understanding the mechanisms through which current methods work and being able to make predictions. In this seminar, I will present my approach to the α -Fe₂O₃ photoanode problem from a first principle perspective. I will show how density functional theory (DFT) and similar quantum mechanical methods can be used in order to understand experimental observations, and make further predictions that enable designing new and improved photocatalyst materials. In particular, I will cover topics that include bulk Pt-doping, α -Al₂O₃ coating surface treatments, and interfaces of α -Fe₂O₃ with FCC metals.

References

1. O. Neufeld and M. Caspary Toroker, "Pt-doped α -Fe₂O₃ for enhanced water splitting efficiency: a DFT+U study", *J. Phys. Chem. C*, 119, 5836, (2015).
2. O. Neufeld and M. Caspary Toroker, "Can we judge an oxide by its cover? The case of platinum over α -Fe₂O₃ from first principles", *Phys. Chem. Chem. Phys.* 17, 24129, (2015).
3. N. Yatom, O. Neufeld, and M. Caspary Toroker, "Toward settling the debate on the role of α -Fe₂O₃ surface states for water splitting", *J. Phys. Chem. C*, 119, (44), 24789, (2015).
4. O. Neufeld, N. Yatom, and M. Caspary Toroker, "A first principles study on the role of an α -Al₂O₃ overlayer on α -Fe₂O₃ for water splitting", *ACS Catal.*, 5, 7237, (2015).

Supervision of Asst. Prof. Maytal Caspary Toroker

ההרצאה תתקיים ביום ראשון, ה- 17 בינואר 2016 בשעה 14:30

באודיטוריום ע"ש דיוויד וואנג, קומה 3, בנין דליה מידן

The lecture will take place on Sunday, January 17th, 2016 at 14:30,

David Wang Auditorium, 3rd floor Dalia Maydan Bldg.

כיבוד קל יוגש לאחר הסמינר