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

Supervision of Asst. Prof. Maytal Caspary Toroker

The lecture will take place on Sunday, January 17th, 2016 at 14:30, David Wang Auditorium, 3rd floor Dalia Maydan Bldg.