

Workshop II: Fuels from Sunlight

Monday October 14, 2013

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Scheffler*
- 9:00–9:15 *Welcome and Opening Remarks*
- 9:15–9:55 **Jens Norskov** (Stanford University)
- 10:15–10:30 *Break*
- 10:30–11:10 **Suljo Linic** (University of Michigan)
Conversion of solar into chemical energy on plasmonic metal nanostructures
- 11:30–11:45 *Break*
- 11:45–12:25 **Bill Schneider** (University of Notre Dame)
Ionic Liquids for Carbon Capture.
- 12:45–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Norskov*
- 2:30–3:10 **Sharon Hammes-Schiffer** (University of Illinois at Urbana-Champaign)
Proton-Coupled Electron Transfer in Catalysis and Energy Conversion
- 3:30–4:00 *Break*
- 4:00–4:40 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday October 15, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Klein*
- 9:00–9:40 **Karsten Reuter** (Technical University Munich (TUM))
Modelling Energy Conversion at Interfaces: Heat and mass transfer effects in in-situ model catalyst studies
- 10:00–10:15 *Break*

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- 10:15–10:55 **John Bell** (Lawrence Berkeley Laboratory)
Fluctuating Navier Stokes Equations for Multicomponent Systems
- 11:15–11:30 *Break*
- 11:30–12:10 **Luca Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Free metal and metal-oxide clusters: beyond the static, monostructure description
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Schuette*
- 2:30–3:10 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)
Fast algorithms for implicit solvation models
- 3:30–4:00 *Break*
- 4:00–4:40 **Yang Shao-Horn** (Massachusetts Institute of Technology)

Wednesday October 16, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Bell*
- 9:00–9:40 **Martin Head_Gordon** (University of California, Berkeley (UC Berkeley))
Electronic structure methods for modeling catalytic processes: Recent advances and applications to proton reduction
- 10:00–10:15 *Break*
- 10:15–10:55 **Reinhold Schneider** (Technische Universität Berlin)
Dynamical low rank approximation in hierarchical tensor formats for electronic structure methods
- 11:15–11:30 *Break*
- 11:30–12:10 **Rupert Klein** (Freie Universität Berlin)
Yserentant's results on the effective complexity of many-electron eigenfunctions
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: G. Galli*
- 2:30–3:10 **Graeme Henkelman** (University of Texas at Austin)
Modeling the structure and activity of nanoparticle catalysts
- 3:30–4:00 *Break*
- 4:00–4:40 **Christof Schuette** (Center for Adaptive Behavior and Cognition)

Thursday October 17, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Reuter*
- 9:00–9:40 **Poul Moses** (Haldor Topsoe)
Computational catalysts design for non-transitional metal catalysts
- 10:00–10:15 *Break*
- 10:15–10:55 **Sohrab Ismail Beigi** (Yale University)
Morphology and electronic alignment of the Poly(3-hexylthiophene)/ZnO interface
- 11:15–11:30 *Break*
- 11:30–12:10 **Norina Richter** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Concentration of Point Defects at Surfaces: The Crucial Role of T, p, and Doping
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Tuckerman*
- 2:30–3:10 **Thomas Bligaard** (Stanford University)
Error estimation and validation of computational trend studies in heterogeneous catalysis
- 3:30–4:00 *Break*
- 4:00–4:40 **Ivano Castelli** (Technical University of Denmark)
High-throughput Screening of New Materials for Water Splitting Applications

Friday October 18, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Henkelman*
- 9:00–9:40 **Eric McFarland** (University of California, Santa Barbara (UC Santa Barbara))
Sustainable Fuels from Sunlight: Start with the Arithmetic
- 10:00–10:15 *Break*
- 10:15–10:55 **Aleksandra Vojvodic** (Stanford University)
- 11:15–11:30 *Break*
- 11:30–12:10 **Richard Hennig** (Cornell University)
Computational Discovery and Design of Two-Dimensional Materials for Energy Technologies

