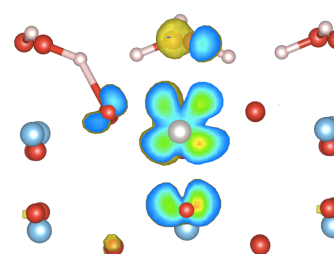
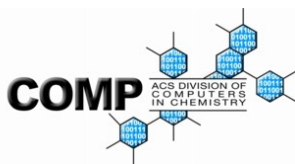




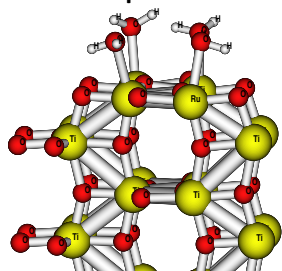
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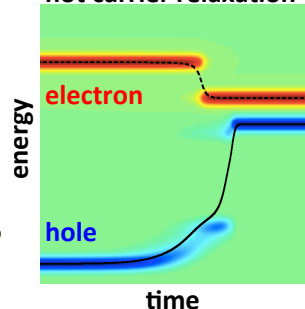
# Computational Photocatalysis - II

This symposium presents current frontiers in computational, experimental and theoretical studies of photoreactions in order to facilitate a synergistic interdisciplinary effort towards computationally assisted design of novel energy materials by addressing two major challenges. Challenge #1 is understanding the basic processes contributing to photo-reactions: light absorption, formation and breaking of charge transfer excitations, hot carrier relaxation, and reaction dynamics at catalytic sites --- all perturbed by environment such as lattice vibrations and solvent polarization and, therefore treated with "open system" approach. Challenge #2 is optimizing efficiency of photo-catalytic and photovoltaic processes by varying the morphology of used nano-materials. Change of composition, quantum confinement, size, shape, surface functionalization, doping, and super-structural arrangements of ordered arrays of nano-crystals provide versatile tuning of timescales of available basic mechanisms and properties of materials. Symposium targets conversion of time-resolved spectroscopic probes and computational descriptions of electronic state and reaction dynamics of nano-structured materials for photo-catalytic and photovoltaic applications.

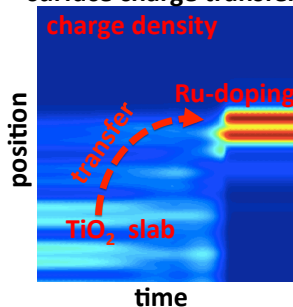
wet & doped surface



hot carrier relaxation



surface charge transfer



## sessions

1. Electronic structure and Excited States
2. Open System Dynamics and Density Matrix
3. Surface hopping and Non-Adiabatic Dynamics
4. Photodissociation theory
5. Photovoltaics and Surface Photovoltage
6. Semiconductor Colloidal Nanorods
7. Semiconductor to metal nanointerface
8. Titanium dioxide surface reactions
9. Time-resolved monitoring of photocatalysis
10. Surface functionalization: doping and dyes
11. Lanthanides and Actinides for solar materials
12. Proton transfer

## Invited Speakers

Giullia Galli (UC Davis)  
Robert Hamers (UWMadison)  
Ranjit Koodali (USD)  
Alan Aspuru-Guzik (Harvard)  
Bruce Parkinson (U Wyoming)  
Ryoji Asahi (Toyota Labs)  
Horia Metiu (UC Santa Barbara)

Oleg Prezhdo (U. of Rochester)  
JR Schmidt (UWMadison)  
Sharon Hammes-Schiffer (Urbana-Champaign)  
Suljo Linic (U. Michigan)  
Donald Truhlar (U. Minnesota)  
James Durrant (Imperial College)  
Martin Head-Gordon (UC Berkeley)

Sergei Tretiak (LANL)  
John T. Yates, jr. (U of Virginia)  
Tim Lian (Emory)  
George Schatz (Northwestern)  
Ladislav Kavan (Heyrovski Inst.)  
Davide Cozzoli (U. del Salento)

David Micha (UFlorida)  
Victor Klimov (LANL)  
James Lewis (UWV)  
Jean-Luc Bredas (GA-Tech)  
Uri Banin (H.U. Jerusalem)  
Victor Batista (Yale)

## International Advisory Committee:

David Micha (UF)  
Ulrike Diebold ([TU Vienna](#))  
Ranjit Koodali (USD)  
Alan Aspuru-Guzik (Harvard)  
Harry B. Gray (Caltech)

Peidong Yang (Berkeley)  
John T. Yates, jr. (U of Virginia)  
Tim Lian (Emory)  
Donald Truhlar (U. Minnesota)  
Kazunari Domen (U. Tokyo)

Annabella Selloni (Princeton University)  
Sharon Hammes-Schiffer (Urbana-Champaign)  
Hrvoje Petek (University of Pittsburgh)  
Uri Banin (H.U. Jerusalem)

**Organizers:** Dmitri Kilin (University of South Dakota), Svetlana Kilina (NDSU), Shuping Huang (USD)

