

## Computational Modeling of Photocatalysis and Photo-induced Charge Transfer Dynamics on Surfaces

Photo-induced dynamics on nano-structured semiconductor surfaces is a rapidly developing area of computational chemistry. Photocatalytic water splitting and Photo-induced Charge Transfer Processes play key roles in renewable energy conversion and storage. 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. We anticipate that discussions at this symposium will lead to new successful collaborations. We expect to facilitate the development of computational methods for correct ab initio description of charge transfer states, photoreactions, and electronic state dynamics induced by interaction with optical perturbations and lattice vibrations. The primary focus is on photovoltaics and photocatalysis at surfaces of semiconductor nano-structures with a broader interest in time-resolved spectroscopic monitoring of related photoreactions.

### INTERNATIONAL ADVISORY COMMITTEE

**John T. Yates, Jr.**  
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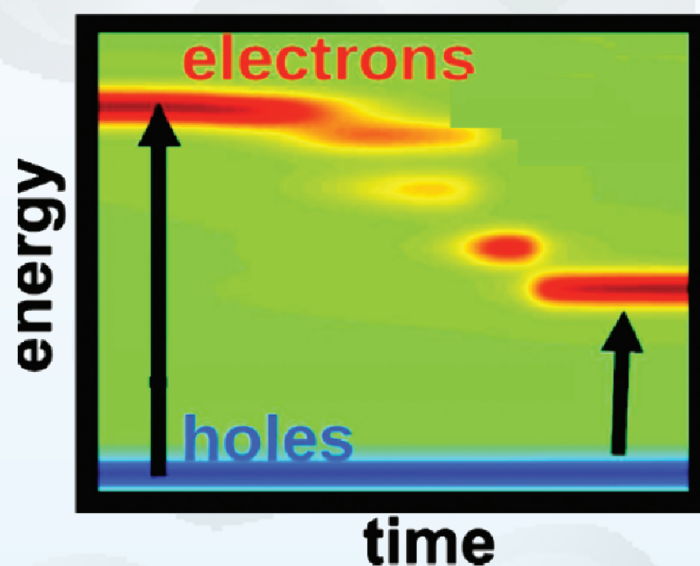
### INVITED SPEAKERS

John T. Yates, Jr., David A. Micha, Daniel G. Nocera, Michael Henderson, Horia Metiu, James Lewis, Prashant Kamat, Victor S. Batista, Giulia Galli, Shao-Chun Li, James Hoefelmeyer, Sergei Tretiak, Oleg Prezhdo, Sharon Hammes-Schiffer, Di Valentino, Stefano Ossicini, Philipp Furche, Charles Schmuttenmaer

**Symposium has 10 half-day sessions, 2 invited and 4 contributed talks per session**

### SESSIONS

- Electronic Structure and Excited States
- Open System Dynamics and Density Matrix
- Surface Hopping and Non-Adiabatic Dynamics
- Photodissociation Theory
- Surface Chemistry of Water
- Surface Photovoltage and Photovoltaics
- Interfaces of Semiconductor Colloidal Nanorods
- Interaction of Plasmonic and Semiconductor Nanoparticles
- Titanium Dioxide Surface Photocatalysis
- Time-Resolved Spectroscopic Monitoring of Photocatalytic Processes
- Doping and Adsorbed Dyes



#### ABSTRACT SUBMISSION INSTRUCTIONS:

- Log into ACS portal; <http://abstracts.acs.org/>
- Navigate to 242nd ACS National Meeting
- Select the program area COMP
- Select symposium, then click "Save"
- Deadline is April 4th

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