INTERNATIONAL ADVISORY COMMITTEE

John T. Yates, Jr.
University of Virginia

David A. Micha
University of Florida

Annabella Selloni
Princeton University

Ulrike Diebold
TU Wien, Vienna, Austria

Ranjit Koodali
University of South Dakota

Victor Batista
Yale

Alán Aspuru-Guzik
Harvard

Martha Symko-Davies
NREL

Hrvoje Petek
University of Pittsburgh

Jürgen Hafner
University of Vienna

Volkhard May
Humboldt-Universität zu Berlin

Ryoji Asahi
Toyota Labs., Inc., Japan

Gustavo E. Scuseria
Rice University

Paul Alivisatos
U.C. Berkeley

George C. Schatz
Northwestern

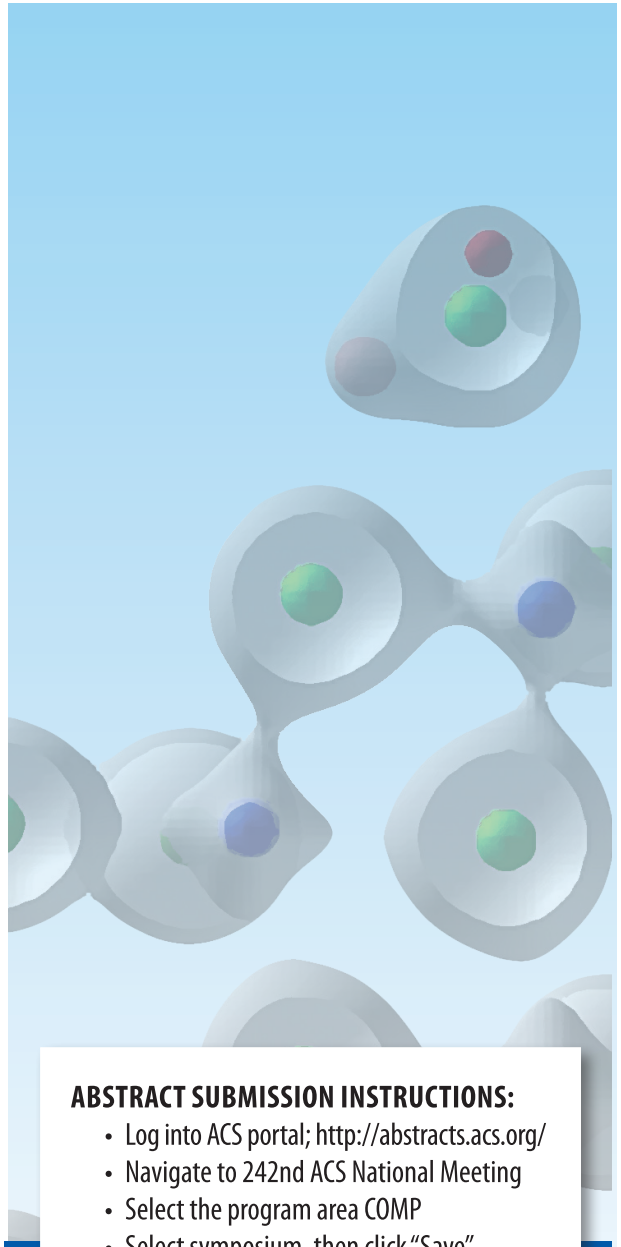
Volkert Eyert
Materials Design, Inc.

Charles Schmuttenmaer
Yale

Thomas Frauenheim
Universität Bremen

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
Cristiana Di Valentin
Stefano Ossicini
Filipp Furche
Charles Schmuttenmaer
Paul Alivisatos
Tania Cuk
Ulrich Ashauer
George C. Schatz
Talgat Inerbaev
Martin Head-Gordon
Tianquan (Tim) Lian
John Asbury



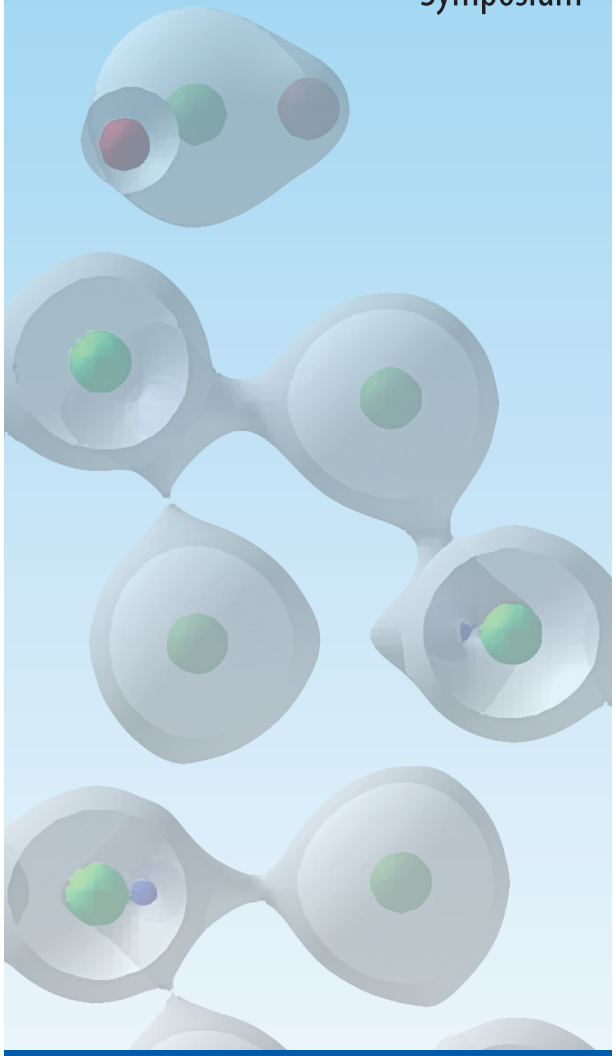
ABSTRACT SUBMISSION INSTRUCTIONS:

- 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

ORGANIZERS:

Dmitri Kilin, Dmitri.Kilin@usd.edu
Svetlana Kilina, Svetlana.Kilina@ndsu.edu
Ivan Mikhaylov, ivan.mikhaylov@gmail.com

242nd ACS National Meeting in Denver, 08/28-09/01, 2011 COMP Division, Symposium



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

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

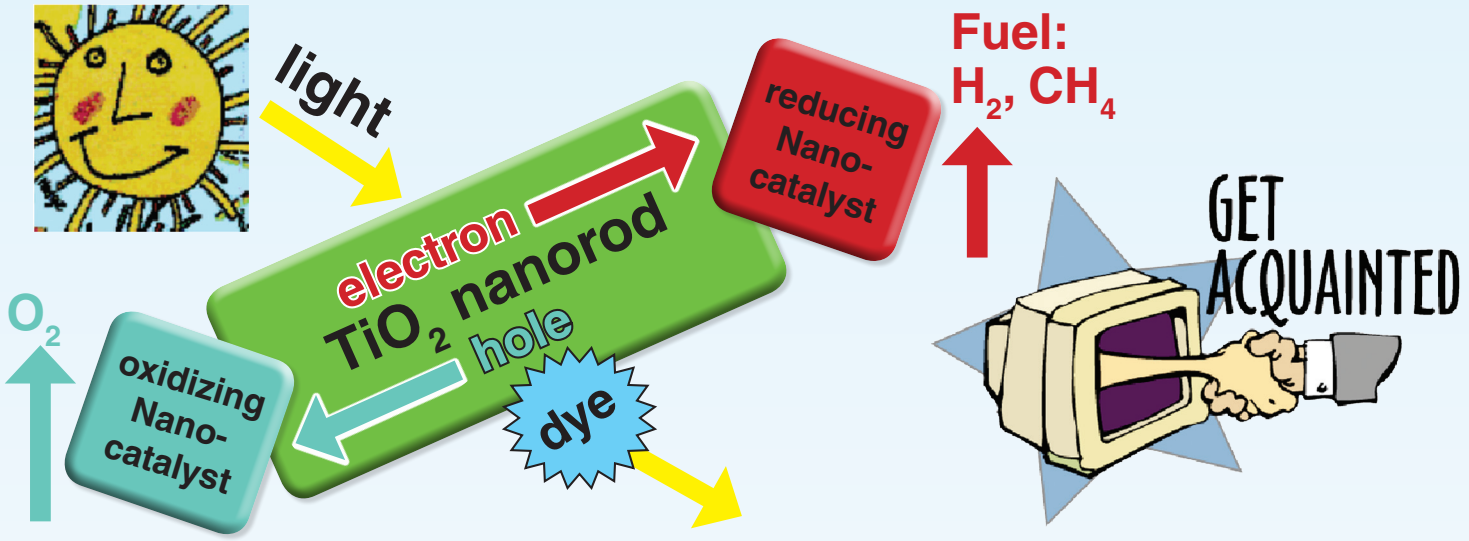


Photo-induced dynamics on nano-structured semiconductor surfaces is a rapidly developing area of computational chemistry. Photocatalytic water splitting and Photo-induced Charge Transfer Processes play key roles in renewable energy conversion and storage. This symposium presents current frontiers in 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 nanostructures with a broader interest in time-resolved spectroscopic monitoring of related photoreactions.

SYMPOSIUM HAS 10 HALF-DAY SESSIONS,

2 invited and 4 contributed talks per session

- 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