Sunday, September 8th, 2013

Session 1: Surface Chemistry for Photocatalysis

Chair: ***D. Kilin***

8:30 am Introductory Remarks

8:35 am **J.Yates, J.Zhang, K. Cao**, *Photo-chemistry on semiconductor surfaces*

9:10 am **R. Asahi**, *Design and development of photocatalytic and photovoltaic materials*

9:45 am **J. Hoefelmeyer**, *Single site metal ions on the surface of TiO_2 nanorods - a platform for theoretical and experimental investigation*

10:10 am INTERMISSION

10:50 am **A. Selloni, YF. Li, J. Chen**, *Mechanism of the first proton coupled electron transfer step in the photo-catalytic oxygen evolution on anatase TiO2: A hybrid Density functional theory*

11:25 am **M. Setvin, P. Scheiber, B. Daniel, M. Fidler, M. Schmid**, ***U. Diebold***, *TiO_2 anatase(101) (sub)surface oxygen vacancies and O_2 adsorption*

11:50 am **X. Gong, W.K. Li, Q. Cuan, Y.Y. Yu**, *DFT calculations of TiO_2 interfaces, surfaces, and catalytic reactions*

Session 2: Charge Transfer Triggers Surface Reactions

Chair: ***Harry Gray and T. Inerbaev***

1:30 pm **A. Akimov, J. Muckerman, O.Prezhdo,** *Non-adiabatic molecular dynamics with time-domain DFT: Theory and applications to photo-voltaic and photocatalytic processes*

2:15 pm **C. Heyes**, *Radiative and nonradiative lifetime engineering of quantum* dots

3:05 pm INTERMISSION

3:20 pm **Z. Han, F. Qiu, R. Eisenberg, P. Holland, T. Krauss**, *Semiconductor nano-crystals for efficient and robust photochemical reduction*

3:55 pm **T. Minegishi, K. Domen**, *Effects of asymmetric surface modification on photoca-talytic particles for sunlight driven water splitting*

4:30 pm INTERMISSION

4:55 pm **S. Hammes-Schiffer**, Non-adiabatic dynamics of photoinduced proton-coupled electron transfer processes

Monday, September 9th, 2013

Session 3: Surface Chemistry for Photocatalysis

Chair: ***A. Kutana***

8:30 am **K. Yamashita**, *Theoretical study on structural and electronic properties of photo-catalytic materials*

9:05 am **J. Christianson, D. Zhu, R. Hamers, J. Schmidt**, *Elucidating the mechanism of reduction of molecular nitrogen by solvated electrons in aqueous solution*

9:30 am **R. Hamers, D. Zhu, J. Christianson, J. Bandy, L. Zhang, J. Schmidt**, *Diamond photo-electron emission into water: A new approach to photo-catalytic reduction of nitrogen reduction at surfaces*

9:55 am **B. Parkinson**, *New oxide semiconductors for water photo-electrolysis: Experimental progress and theoretical issues*

10:30 am INTERMISSION

10:45 am **G. Galli**, *Electronic excitations in light absorbers for photoelectrochemical energy conversion: First principles calculations based on many body perturbation theory*

11:20 am **M. Dawber, B. Bein**, *Engineered ferro-electric surfaces for photocatalysis*

11:45 am **M. Fernandez-Serra, P. Allen, J. Liu, L. Pedroza**, *Water structure and redox level alignment at the water-semiconductor interface from first principles*

Session 4: Surface Chemistry for Photocatalysis

Chair: ***A. Akimov***

1:30 pm **E. McFarland, H. Metiu**, *Catalytic chemistry of doped reducible oxides*

2:05 pm **S.K. Parayil, H. Kibombo, CM. Wu, J. Baltrusaitis, R. Koodali**, *Influence of oxidation state of platinum on TiO_2 for solar simulated photocatalytic hydrogen production from H_2O*

2:30 pm **T. Inerbaev, J. Hoefelmeyer, D. Kilin,** *Effect of doping on thermodynamic stability and electronic properties of bulk and nanotitania*

2:55 pm **J. Lewis**, *High-throughput compu-tational design of photo-catalytic materials*

3:20 pm INTERMISSION

3:35 pm **Y. Sun**, *Water splitting with TiO2: Band gap engineering and catalytic role of photoholes*

Monday, September 9th, 2013

4:00 pm **S. Fischer, J. May, X. Li**, *Non-adiabatic molecular dynamics investigation of charge transfer state formation in Mn(II)-doped ZnO quantum dots*

4:35 pm **A. Kutana, D. Kilin**, *Charge dissipation in doped quantum dots*

5:00 pm **J. McCusker**, Ultrafast excited-state processes of first-row transition metal complexes: Challenges and opportunities in solar energy conversion

Tuesday, September 10th, 2013

Session 5: Interface Charge Transfer and Dye-Sensitized Solar Cells

Chairs: ***A. Kryjevski***

8:30 am **V. Batista**, *Computational inverse design of photocatalysts for renewable energy*

9:05 am **F. De Angelis, M. Pastore**, *Modeling materials & process in dye-sensitized solar cells*

9:30 am **G. Sereda, R. Koodali, C. Marshall, R. Peng, S. Banerjee, T. Kim, H. Subramanian, A. Jones, H. Khatri**, *Deposition of vanadia- and titania-catalysts on solid supports using macro-cyclic organic templates*

9:55 am **S. Konezny, C. Richter, D. Talbayev, R. Snoeberger, R. Crabtree, V. Batista, G. Brudvig, C. Schmuttenmaer**, *Using the fluctuation-induced tunneling conduction model for describing and understanding bulk charge transport in nano-structured materials*

10:30 am INTERMISSION

10:45 am **J. Neaton**, *Theory of organic ad-sorbate frontier orbital energies on functionali-zed light-absorbing semiconductor surfaces*

11:10 am **P. Deak, B. Aradi, T. Frauenheim**, *Peculiarities of TiO_2: Carrier self-trapping and massless electron states*

11:35 am **Y. Dahnovsky, A. Pimachev, V. Proshchenko**, *Fast electron dynamics in QD sensitized solar cells: Two approaches*

Tuesday, September 10th, 2013

Session 6: Nanostructures for Photovoltaics

Chair: ***S. Kilina***

1:30 pm **V. Klimov**, *Carrier multiplication in semiconductor nanocrystals within the framework of two competing energy relaxation mechanisms*

2:05 pm **K. Hyeon-Deuk**, *Photoexcited hole and electron dynamics coupled to phonon modes in semiconductor quantum dots*

2:30 pm **Y. Yang, T. Lian**, Efficient multiple exciton dissociation and hot electron extraction from PbS QD

2:55 pm **A. Kryjevski, S. Kilina, D. Kilin**, *Photo-excitations in arrays of semiconductor quantum dots: DFT computation*

3:20 pm INTERMISSION

3:35 pm **E. Rabani**, *Metastability in pressure-induced structural transformations of core/shell nanocrystals*

4:10 pm **T. Lian**, *Solar-to-fuel conversion using artificial atoms, molecules, and solids*

4:45 pm **J. Asbury**, *Stokes shifted electron transport states in quantum dot solids*

Wednesday, September 11th, 2013

Session 7: Organic Semiconductors and Biosystems

Chair: ***E. Jakubikova***

8:30 am Introductory Remarks

8:35 am **JL. Bredas**, *Electronic and geometric structure of hybrid oxide-organic interfaces of relevance to OLED and OPV devices*

9:10 am **S. Tretiak**, *Localization of electronic excitations in organic semiconductors: Theoretical views from different angles*

9:35 am **H.P. Cheng, I.C. Chu, D. Kilin**, *First-principles studies of photoinduced charge transfer in functionalized carbon nanotubes*

10:00 am **A. Aspuru-Guzik**, *Light harvesting in green sulfur bacteria: Entire apparatus com-putational studies of excitonic energy transfer*

10:25 am INTERMISSION

10:40 am **M. Caricato, F. Lipparini, C. Cappelli, V. Barone,** *Absorption spectra in solution with the EOM-CCSD method and a classical polarizable explicit-implicit solvation model*

11:05 am **C. Isborn, V. Tung, A. Martini, E. Johnson**, *Computing excited states in aqueous solution and nanocarbon photovoltaics: Chirality is key to efficiency*

Wednesday, September 11th, 2013

Session 8: Plasmonic Materials and Nano-Interfaces

Chair: ***S. Tretiak***

1:30 pm **G. Schatz**, *Modeling excited state dynamics in nanoparticles and nanocrystals*

2:05 pm **R. Schaller**, *Probing carrier and lattice dynamics in semiconductor nanocrystals and semiconductor-metal hybrids*

2:30 pm **U. Banin**, *Light induced charge separation and photocatalysis in hybrid semiconductor-metals* nanostructures

3:05 pm **K. Wu, H. Zhu, T. Lian**, *Plasmon-induced broadband light harvesting and charge separation in CdS-Au nanoheterostructures*

3:30 pm INTERMISSION

3:45 pm **S. Linic**, *Chemical transformations with optically excited plasmonic nanoparticles from first principles*

4:20 pm **C. Liu, J. Tang, N. Dasgupta, P. Yang,** Nanowire-based structures for solar-to-fuel conversion

Thursday, September 12th, 2013

Session 9: Single-Site Transition Metal Photocatalysis and Non-adiabatic Dynamics

Chair: ***D. Kilin***

8:30 am **J. Panetier, M. Head-Gordon**, *Modeling molecular electro-catalysts for proton and CO_2 reduction*

9:05 am **H. Petek, L. Peker, M. Feng, H. Sun, J. Zhao**, Atomic scale imaging of CO_2 capture by metal-organic frameworks

9:30 am **E. Jakubikova**, *Adventures in computational design of chromophores: Can we replace ruthenium in Ru(II)-polypyridines with iron?*

9:55 am **D. Micha**, *Modeling photoconductivity at a semiconductor surface: An application to nano-structured Si surfaces*

10:30 am INTERMISSION

10:45 am **D. Truhlar**, *Electronic structure of excited states for nonadiabatic dynamics*

11:20 am **D. Mozyrsky**, *Semiclassical Monte-Carlo approach for modeling non-adiabatic dynamics in extended molecules*

11:45 am **J. Parkhill**, *Fast, atomistic bath models for electronic dynamics applied to charge separation in zeolites*

ACS 246th National Meeting

Division of Computers in Chemistry

Symposium: Computational Photo-catalysis II

Organizers: Dmitri Kilin, Svetlana Kilina, and Shuping Huang

Sunday, September 8th, – Thursday, September 12th, 2013

Indiana Convention Center, Room 138

Sunday 9/8/13

Session #1: Surface Chemistry for Photo-catalysis

Session #2: Charge Transfer Triggers Surface Reactions

Monday 9/9/13

Session #3: Surface Chemistry for Photo-Catalysis (cont.)

Session #4: Surface Chemistry for Photo-Catalysis (cont)

Tuesday 9/10/13

Session #5: Interface Charge Transfer and Dye-Sensitized Solar Cells

Session #6: Nanostructures for Photo-Voltaics

Wednesday 9/11/13

Session #7: Organic Semiconductors and Biosystems

Session #8: Plasmonic Materials and Nano-Interfaces

Thursday 9/12/13

Session #9: Transition Metal Photocatalysis and Non-adiabatic Dynamics
