

Wednesday Morning
Novel Concepts for Solar Energy Conversion
John Asbury, Presiding

8:30 (264). Harvesting singlet fission for solar energy conversion: Charge vs. energy transfer, **Xiaoyang Zhu**

9:10 (265). Solar energy harvesting and photoinduced charge separation at TiO₂ interfaces: Insights from time-domain ab initio simulations, **Oleg Prezhdo**

9:50 (266). Lessons from carotenoid assemblies for exciton fission, and their connection to solar energy conversion, **Michael J. Tauber**, Chen Wang, Maria Angelella, Samantha J. Doyle, Christopher J. Berg

10:10 INTERMISSION

10:30 (267). Singlet fission and triplet exciton dynamics in organic semiconductors, **Chris Bardeen**, Jon Burdett, Robert Dillon, Geoff Piland, Valerie Nichols, Jiun-Haw Lee

11:10 (268). Theory-aided design of OPV's: Molecular choice, entropy, charge guidance, and collection, **Mark Ratner**, Brett Savoie, Tobin Marks

11:50 (269). Solar vapor generation enabled by nanoparticles, Naomi J. Halas, **Oara Neumann**, Alex Urban, Nathaniel Hogan, Zheyu Fang, Alberto Pimpinelli, Surbhi Lal, Peter Nordlander

Wednesday Afternoon
Emerging Techniques for Solar Energy Conversion
Clifford Kubiak, Presiding

1:30 (300). Ultrafast studies of charge carrier trapping in single semiconductor nanowires, Shun S Lo, Mary Sajini Devadas, Todd A Major, **Gregory V Hartland**

2:10 (301). Charge and exciton migration in carbon nanotube and dye sensitized solar cells using 2D spectroscopies, **Martin Zanni**

2:50 (302). Vibrational relaxation of N3 at single crystalline TiO₂ surfaces, Carmella Calabrese, Heather Vanselow, **Poul B Petersen**

3:10 INTERMISSION

3:30 (303). Structural dynamics of transition metal complexes in photocatalytic reactions for solar energy conversion, **Lin X. Chen**

4:10 (304). Investigating the role of orientation and order in charge transport at organic interfaces by nonlinear spectroscopy, **Aaron M. Massari**

4:50 (305). Light harvesting in photosynthesis: Insights gained from 2D electronic spectroscopy, **Jessica M. Anna**, Gregory D. Scholes

Thursday Morning
Interfacial Electron Transfer: Frank Willig Memorial Symposium
Bruce Parkinson, Lars Gundlach, Mark Spitler, Presiders

8:30 am. Introductory Remarks

8:50 (536). Photosensitization of semiconductor electrodes: Collaborations with Frank Willig, **Bruce Parkinson**

9:10 (537). Time scales for electron transfer in dye sensitized systems, **Mark T. Spitler**

9:30 (538). Spectra for ultrafast photoinduced heterogeneous electron transfer reveal importance of high energy vibrational modes, **Lars Gundlach**

9:50 (539). Energetics and dynamics of heterogeneous interfacial electron transfer reactions: A complementary time resolved study, **Rainer Eichberger**, Klaus Schwarzburg, Thomas Hannappel

10:10 (540). Chemical control of heterogeneous electron transfer dynamics and strong electron-lattice coupling in TiO₂, **Ralph Ernstorfer**

10:30 INTERMISSION

10:50 (541). Molecular design of dyes for dye/metal oxide charge transfer interfaces: An overview and new directions, **Elena Galoppini**

11:10 (542). Quantum photoelectrochemical predictions of nanoscale solar energy conversion properties, **Petter Persson**, Svante Hedström, Marta Knitter, Tomas Österman

11:30 (543). Ultrafast dynamics of interfacial electron transfer, **Martin Wolf**

11:50 (544). Plasmon enhancement of charge and energy transfer in nanohybrid-systems, **Volkhard May**, Luxia Wang

12:10 (545). Excited state dynamics of P3HT in close proximity to nanostructured metal surfaces, Jianhua Bao, Zhihao Yu, Lars Gundlach, Deirdre O'Carroll, **Piotr Piotrowiak**

Thursday PM, Novel Concepts for Solar Energy Conversion
Oleg Prezhdo, Presiding

1:30 (562). Harvard Clean Energy Project: High-throughput screening and design of organic photovoltaic materials via automated, first-principles quantum chemistry on the IBM World Community Grid, **Johannes Hachmann**, Roberto Olivares-Amaya, Sule Atahan-Evrenk, Alan Aspuru-Guzik

1:50 (563). Elucidation of the photodynamics of single LH2 proteins in solution, **Gabriela S. Schlau-Cohen**, June Southall, Richard J. Cogdell, William E. Moerner

2:10 (564). WITHDRAWN

2:30 (565). 1,3-Diphenylisobenzofuran as an archetype for studies of singlet fission, **Joel Schrauben**, Joe Ryerson, Justin Johnson

2:50 (566). Molecular modeling of singlet fission in dye sensitized solar cells, Ulyana S. Cubeta, Edward Ko, **Hanning Chen**

3:10 (567). Structural characteristics and dynamics of excited conjugated polymers probed by time-resolved Raman spectroscopy, **Arthur E Bragg**

3:30 (568). Exciton dissociation at phthalocyanine-C₆₀ interfaces, G. J. Dutton, **S. W. Robey**

3:50 (569). Effects of side-chain structure and electronic structure of p-type polymer on the photovoltaic properties of organic solar cells, **Samson A. Jenekhe**, Guoqiang Ren, Selvam Subramaniyan, David S. Ginger, Cody W. Schlenker

4:10 (570). Simulations of delocalization and morphology effects on charge and exciton transport in organic photovoltaics, **Geoffrey R Hutchison**, Adam G Gagorik

246th National ACS Meeting

Division of Physical Chemistry

Physical Chemistry of Solar Energy Conversion

R. Brian Dyer
Tianquan (Tim) Lian

Organizers

Indiana Convention Center
Room 239

September 8-12, 2013

Sunday Morning

Quantum Dots and Nanorods for Solar Energy Conversion

Tim Lian, Presiding

8:30 (1). Multiple exciton generation and carrier dynamics in PbSe and Si QDs, QD films, and doped PbSe QDs, **Matthew C. Beard**, Aaron G. Midgett, Barbara K. Hughes, Joseph M. Luther, Arthur J. Nozik
9:10 (2). Semiconductor nanocrystals and solar energy conversion, **Victor I. Klimov**
9:50 (3). Effect of heterojunction on exciton dissociation in core/shell quantum dots, **Arindam Chakraborty**
10:10 INTERMISSION
10:30 (4). Thermal activation of the Auger processes in charged CdSe/CdS core/shell NCs, Alexander Efros, Benoit Mahler, Benoit Dubertret, C. Javaux, **Andrew Shabaev**, Anna Rodina, D. R. Yakovlev, F. Liu, M. Bayer, L. Biadala, S. Buil, X. Quelin, J.-P. Hermier
11:10 (5). Spontaneous multi-electron transfer from the surfaces of PbS quantum dots to TCNQ, Kathryn E. Knowles, Michal Malicki, Radha Parameswaran, Laura C. Cass, **Emily A. Weiss**
11:50 (6). Full-spectrum solar cells based on colloidal quantum dots: Advances in materials chemistry and impact on photovoltaic device performance, **Edward H. Sargent**

Sunday Morning

Artificial Photosynthesis: Water Oxidation

R. Brian Dyer, Presiding

1:30 (45). Studies of oxomanganese complexes for natural and artificial photosynthesis, **Victor S Batista**
2:10 (46). Co oxide nanotubes as water oxidation catalysts in artificial photosynthetic units, **Heinz M Frei**
2:50 (47). Mid-gap, infrared crystal field transitions as efficient electron trap states in Co₃O₄ with implications for the water oxidation reaction, **Tanja Cuk**, Matthias Waagele, Hoang Doan
3:10 INTERMISSION
3:30 (48). Water oxidation in natural and artificial photosynthesis studied using X-ray spectroscopy, **Junko Yano**, Jan Kern, Vittal Yachandra
4:10 (49). Water oxidation chemistry of Photosystem II and artificial systems, **Gary W Brudvig**
4:50 (50). Forming junctions at the nanoscale for improved solar water splitting, Matt Mayer, Chun Du, Rui Liu, Carrie Stephani, **Dunwei Wang**

Monday Morning

Quantum Dots and Nanorods for Solar Energy Conversion

Emily Weiss, Presiding

8:30 (89). Research in solar photoconversion at DOE Basic Energy Sciences, **Mark T. Spitler**
9:10 (90). Studies of structure, doping, and transport in quantum dot arrays, **A. Paul Alivisatos**
9:50 (91). Efficient solar-to-fuel conversion using quantum confined semiconductor nanoheterostructures, **Haiming Zhu**, Tianquan Lian
10:10 INTERMISSION
10:30 (92). Design of solution-processed semiconductors from colloidal nanocrystals for photovoltaics and thermoelectrics, Chengyang (Raymond) Jiang, Jae Sung Son, Wenyong Liu, Jaeyoung Jang, **Dmitri V Talapin**
11:10 (93). Designing tandem layered quantum dot solar cells with CdSeS nanocrystals, **Prashant V. Kamat**, Pralay Santra
11:50 (94). How to dope a semiconductor nanocrystal?, **Uri Banin**

Monday Afternoon

Artificial Photosynthesis: Solar Fuels

Gary Brudvig, Presiding

1:30 (132). Carbon dioxide reduction by rhenium and manganese bipyridyl complexes: Mechanistic insights, **Clifford P. Kubiak**
2:10 (133). From CO₂ hydrogenation by solar produced H₂ to photochemical water oxidation, **Etsuko Fujita**, Yosra M Badiei, Wei-Fu Chen, Anna Lewandowska-Andralojc, James T Muckerman, Dmitry E Polyansky, Kotaro Sasaki, Wan-Hui Wang, Yuichiro Himeda
2:50 (134). Demonstration of artificial photosynthesis with peeled silicon microrod arrays, **Shane Ardo**, Chris W. Roske, Emily L. Warren, Bruce S. Brunschwig, Harry A. Atwater, Nathan S. Lewis
3:10 INTERMISSION
3:30 (135). Robust photogeneration of H₂ in water using semiconductor nanocrystals and a nickel catalyst, Fen Qiu, Zhiji Han, Richard Eisenberg, Patrick L. Holland, **Todd D. Krauss**
4:10 (136). Non-innocence of the electrode interface in low overpotential reduction of CO₂ to organic products, **Andrew Bocarsly**, Jing Gu, Yong Yan, John Watkins, Elizabeth Zeitler, Zachary Detweiler, Yuan Hu, Kuo Liao, James White, Maor Baruch, James Pander, Anna Wuttig
4:50 (137). Quantum mechanical insights into photoelectrochemical CO₂ reduction processes, **John A Keith**, Emily A. Carter

Tuesday Morning

Organic Solar Cells

Todd Krauss, Presiding

8:30 (175). Charge separation and recombination in organic solar cells, **James R Durrant**
9:10 (176). Electronic and optical processes in organic solar cells: Insights from a multiscale computational approach, **Jean-Luc Bredas**
9:50 (177). Exciton diffusion in long-chain organic conjugated molecules, **Adam P Willard**, Peter J Rossky
10:10 INTERMISSION
10:30 (178). Controlling nm-scale morphology in bulk heterojunction solar cells: Self-assembling polymers and fullerenes and sequential processing, **Benjamin J. Schwartz**
11:10 (179). Ultrafast infrared spectroscopy of charge generation, trapping, and transport in emerging photovoltaic materials, **John B. Asbury**
11:50 (180). Uncovering vibrational dynamics and charge transfer interactions with resonance Raman spectroscopy, **John Grey**, Jian Gao, **John Grey**, Jian Gao, Adam Wise

Tuesday Afternoon

Artificial Photosynthesis: Solar Fuels

Clifford Kubiak, Presiding

1:30 (219). Photoinduced charge transport in self-assembled nanostructures for solar energy conversion, **Michael R Wasielewski**, Vladimir Roznyatovskiy, Yi-Lin Wu
2:10 (220). Artificial photosynthesis and bio-inspired solar-to-fuel strategies, **Benjamin Sherman**, Thomas A. Moore, Devens Gust, Ana L. Moore, Thomas E. Mallouk
2:50 (221). Quantum dynamics from classical trajectories: New approaches to simulating biological and molecular photocatalysts, **Thomas F Miller**
3:10 INTERMISSION
3:30 (222). Excited state dynamics and solar photochemistry of semiconductor nanocrystals, Molly Wilker, Katherine Brown, Huan-Wei Tseng, Niels Damrauer, Paul King, **Gordana Dukovic**
4:10 (223). Solar hydrogen-producing bionanodevice that outperforms natural photosynthesis, Carolyn E Lubner, Amanda M Applegate, Philipp Knorzer, Alexander Ganago, Donald A Bryant, Thomas Happe, **John H Golbeck**
4:50 (224). Control of photocatalytic hydrogen production in enzyme-nanoparticle assemblies, Katherine A Brown, Molly B Wilker, David W Mulder, Qing Song, Gordana Dukovic, **Paul W King**