

## Session Index

### Session M2: Focus Session: Charge & Energy Transfer I

Sponsoring Units: DCP

Chair: Nathan Gabor, Massachusetts Institute of Technology

Room: 102

Wednesday, March 5, 2014 11:15AM - 11:51AM	<a href="#">M2.00001: The optoelectronic properties of in-plane grain boundaries and out-of-plane interfaces in two-dimensional transition metal dichalcogenides</a> Invited Speaker: Arend van der Zande
Wednesday, March 5, 2014 11:51AM - 12:03PM	<a href="#">M2.00002: Photosynthesis Revisited: Optimization of Charge and Energy Transfer in Quantum Materials</a> Nathaniel Gabor
Wednesday, March 5, 2014 12:03PM - 12:15PM	<a href="#">M2.00003: Charge and spin transport in porphyrin-based molecular junctions</a> Zhenfei Liu , Sujun Wei , Olgun Adak , Hongsik Yoon , Luis M. Campos , Woo-Dong Jang , Latha Venkataraman , Jeffrey B. Neaton
Wednesday, March 5, 2014 12:15PM - 12:27PM	<a href="#">M2.00004: Two Dimensional White Light Spectroscopy Reveals Energy Transfer Pathways in Semiconducting Carbon Nanotube Thin Films</a> Randy Mehlenbacher , Thomas McDonough , Maksim Grechko , Nicholas Kearns , Meng-Yin Wu , Michael Arnold , Martin Zanni
Wednesday, March 5, 2014 12:27PM - 1:03PM	<a href="#">M2.00005: Optoelectronics of Two-Dimensional Transition Metal Dichalcogenides</a> Invited Speaker: Xiaodong Xu
Wednesday, March 5, 2014 1:03PM - 1:15PM	<a href="#">M2.00006: Energy Level Alignment for Many-Body Resonant Tunneling</a> Jessica Walkenhorst , Heiko Appel , Nicole Helbig , Angel Rubio
Wednesday, March 5, 2014 1:15PM - 1:27PM	<a href="#">M2.00007: Probing Transport through Single Molecule Junctions by Electrolytic Gating</a> Brian Capozzi , Q. Chen , P. Darancet , M. Buzzeo , J.B. Neaton , C. Nuckolls , L. Venkataraman
Wednesday, March 5, 2014 1:27PM - 1:39PM	<a href="#">M2.00008: Projection operators - non-equilibrium Green functions approach to quantum transport</a> Maicol Ochoa , Michael Galperin , Mark Ratner
Wednesday, March 5, 2014 1:39PM - 2:15PM	<a href="#">M2.00009: Optical Properties of Two-Dimensional Crystals and Heterostructures</a> Invited Speaker: Feng Wang

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### Session Q1: Focus Session: Charge & Energy Transfer II

Sponsoring Units: DCP

Chair: Xiaoyang Zhu, Columbia University

Room: 103/105

Wednesday, March 5, 2014 2:30PM - 3:06PM	<a href="#">Q1.00001: Optical Excitation and Energy Relaxation in Graphene: Layer by Layer</a> Invited Speaker: Jiwoong Park
Wednesday, March 5, 2014 3:06PM - 3:18PM	<a href="#">Q1.00002: Understanding the charge-transfer phenomena between prototypical electron-donors and acceptors: TTF-TCNQ as an example</a> Changwon Park , Viktor Atalla , Sean Smith , Mina Yoon
Wednesday, March 5, 2014 3:18PM - 3:30PM	<a href="#">Q1.00003: Fast electron transfer at molecule-substrate interfaces</a> Guido Fratesi , Carlo Motta , Mario Italo Trioni , Daniel Sanchez-Portal , Gian Paolo Brivio
Wednesday, March 5, 2014 3:30PM - 3:42PM	<a href="#">Q1.00004: Non-adiabatic vibrational-electronic resonance in a model dimer - Implications for Photosynthetic Energy Transfer</a> Vivek Tiwari , David Jonas
Wednesday, March 5, 2014 3:42PM - 4:18PM	<a href="#">Q1.00005: Dynamics of electron transfer and exciton formation at interfaces</a> Invited Speaker: Martin Wolf
Wednesday, March 5, 2014 4:18PM - 4:30PM	<a href="#">Q1.00006: Modeling recombination processes and predicting energy conversion efficiency of dye sensitized solar cells from first principles</a> Wei Ma , Sheng Meng
Wednesday, March 5, 2014 4:30PM - 4:42PM	<a href="#">Q1.00007: Tunable Band Edges of TiO<sub>2</sub> via Functionalization with Phosphonic Acid Adsorbates</a> Guo Li , Jessy Rivest , Ian Sharp , Delia Milliron , Jeffrey Neaton
Wednesday, March 5, 2014 4:42PM - 4:54PM	<a href="#">Q1.00008: A novel theoretical probe of the SrTiO<sub>3</sub> surface under water-splitting conditions</a> Kendra Letchworth-Weaver , Deniz Gunceler , Tom\as Arias , Manuel Plaza , Xin Huang , Joel Brock , Joaquin Rodriguez-L\opez , Hector Abru\~na
Wednesday, March 5, 2014 4:54PM - 5:30PM	<a href="#">Q1.00009: Efficient Plasmon-Induced Hot Electron Transfer and Photochemistry in Semiconductor-Au Nanorod Heterostructures</a> Invited Speaker: Tianquan Lian

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### Session S1: Focus Session: Charge & Energy Transfer III

Sponsoring Units: DCP

Chair: Martin Wolf, Fritz-Haber-Institute

Room: 103/105

Thursday, March 6, 2014 8:00AM - 8:12AM	<a href="#">S1.00001: First-principles calculation of photo-induced electron transfer rate constants in phthalocyanine-C<sub>60</sub> organic photovoltaic materials: Beyond Marcus theory</a> Myeong H. Lee , Barry D. Dunietz , Eitan Geva
Thursday, March 6, 2014 8:12AM - 8:24AM	<a href="#">S1.00002: Exciton dissociation at phthalocyanine-C<sub>60</sub> interfaces</a> S.W. Robey , G.J. Dutton
Thursday, March 6, 2014 8:24AM - 8:36AM	<a href="#">S1.00003: Passive exciton gating via directed energy transfer in organic photovoltaic cells</a> S. Matthew Menke , Tyler K. Mullenbach , Russell J. Holmes
Thursday, March 6, 2014 8:36AM - 9:12AM	<a href="#">S1.00004: Direct observation of ultrafast long-range charge separation at polymer:fullerene heterojunctions</a> Invited Speaker: Carlos Silva
Thursday, March 6, 2014 9:12AM - 9:24AM	<a href="#">S1.00005: Exploring the Influence of Dynamic Disorder on Excitons in Solid Pentacene</a> Zhiping Wang , Sahar Sharifzadeh , Peter Doak , Zhenfei Lu , Jeffrey Neaton
Thursday, March 6, 2014 9:24AM - 9:36AM	<a href="#">S1.00006: Singlet fission in reduced dimensions of crystals</a> Paul Teichen , Joel Eaves
Thursday, March 6, 2014 9:36AM - 9:48AM	<a href="#">S1.00007: Fission of Entangled Spins: An Electronic Structure Perspective</a> Xintian Feng , Anatoliy Luzanov , Anna Krylov
Thursday, March 6, 2014 9:48AM - 10:24AM	<a href="#">S1.00008: Exciton fission, dissociation and transport in organic conjugated materials: Modeling insights</a> Invited Speaker: David Beljonne
Thursday, March 6, 2014 10:24AM - 10:36AM	<a href="#">S1.00009: First Principles Calculations of Conformational and Electronic Properties of PTB7</a> Ram Bhatta , David Perry , Mesfin Tsige
Thursday, March 6, 2014 10:36AM - 10:48AM	<a href="#">S1.00010: Understanding the Role of Orientational Heterogeneity on Photophysical Properties of Organic Polycrystalline Films</a> Sahar Sharifzadeh , Cathy Wong , Hao Wu , Naomi Ginsberg , Leeor Kronik , Jeffrey Neaton
Thursday, March 6, 2014 10:48AM - 11:00AM	<a href="#">S1.00011: Theoretical Modeling and Design of Organic Semiconductors with High Carrier Mobility</a> Xiao Ma , Changhua Zhen , John Kieffer

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### Session W1: Focus Session: Charge & Energy Transfer IV

Sponsoring Units: DCP

Chair: Carlos Silva, University of Montreal

Room: 103/105

Thursday, March 6, 2014  
2:30PM - 2:42PM

[W1.00001: Carrier dynamics in colloidal indium arsenide quantum dots in the weak excitation limit](#)

Austin Spencer , William Peters , Vivek Tiwari , Byungmoon Cho , Nathan Neale , David Jonas

Thursday, March 6, 2014  
2:42PM - 2:54PM

[W1.00002: Photoinduced Electron Transfer to Engineered Surface Traps in CdSe Nanocrystals](#)

Marco Califano , Haiming Zhu , Ye Yang , Kim Hyeon-Deuk , Nianhui Song , Youwei Wang , Wenqing Zhang , Oleg Prezhdo , Tianquan Lian

Thursday, March 6, 2014  
2:54PM - 3:06PM

[W1.00003: Electron - acoustic phonon coupling in colloidal lead sulfide quantum dots](#)

Byungmoon Cho , Vivek Tiwari , Austin Spencer , Dmitry Baranov , Samuel Park , David Jonas

Thursday, March 6, 2014  
3:06PM - 3:42PM

[W1.00004: Engineered semiconductor nanocrystals with enhanced carrier multiplication yields](#)

Invited Speaker: Victor Klimov

Thursday, March 6, 2014  
3:42PM - 3:54PM

[W1.00005: Characterization and 2D FT electronic spectra of colloidal PbSe nanocrystals](#)

Dmitry Baranov , Samuel Park , Byungmoon Cho , David Jonas

Thursday, March 6, 2014  
3:54PM - 4:06PM

[W1.00006: Single Molecule Spectroscopy and Scanning Probe Microscopy to Investigate Excited State Energy Transport in Quantum Dot Higher Order Structures](#)

Alan Van Orden , Martin Gelfand , Duncan Ryan , Kevin Whitcomb

Thursday, March 6, 2014  
4:06PM - 4:18PM

[W1.00007: Breaking the symmetry of a PbSe quantum dot by a hot electron-hole pair](#)

Minh-Tuan Trinh , Xiaoyang Zhu

Thursday, March 6, 2014  
4:18PM - 4:54PM

[W1.00008: Multiexciton Generation in Nanocrystals and Nanorods](#)

Invited Speaker: Eran Rabani

Thursday, March 6, 2014  
4:54PM - 5:06PM

[W1.00009: Multiple exciton generation and singlet fission: the role of collective effects](#)

Joel Eaves , Mark Sweeney , Paul Teichen , Steven Strong

Thursday, March 6, 2014  
5:06PM - 5:18PM

[W1.00010: Hierarchical Equation of Motion Investigation of Decoherence and Relaxation Dynamics in Nonequilibrium Transport through Interacting Quantum Dots](#)

Rainer Hartle , Guy Cohen , David R. Reichman , Andrew J. Millis

Thursday, March 6, 2014  
5:18PM - 5:30PM

[W1.00011: Studying the Photoexcitation Quenching Mechanism in Quantum Dot-Nitroxide Radical Hybrid Systems](#)

Poulami Dutta , Jeffrey Sayen , Remi Beaulac

## Session Index

### Session Y2: Focus Session: Charge & Energy Transfer V

Sponsoring Units: DCP  
Chair: Tim Lian, Emory University  
Room: 102

Friday, March 7, 2014 8:00AM - 8:12AM	<a href="#">Y2.00001: Bipolar Charge Transport Properties of Poly(imide-thienyl(thienylenevinylene))</a> Evan Lafalce , Xiaomei Jiang , Cheng Zhang
Friday, March 7, 2014 8:12AM - 8:24AM	<a href="#">Y2.00002: A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions</a> Tamar Zelovich , Leeor Kronik , Oded Hod
Friday, March 7, 2014 8:24AM - 8:36AM	<a href="#">Y2.00003: Femtosecond Nonlinear Optical Studies of Radiationless Decay in Carotenoids and in the Peridinin--Chlorophyll <math>a</math> Protein</a> Soumen Ghosh , Michael Bishop , Jenny Jo Mueller , Nolan Shepherd , Warren Beck , Harry Frank
Friday, March 7, 2014 8:36AM - 9:12AM	<a href="#">Y2.00004: Energy and Charge Transfer in Dinuclear Ru-based Complexes</a> Invited Speaker: Valeria Kleiman
Friday, March 7, 2014 9:12AM - 9:24AM	<a href="#">Y2.00005: Optical Excitations in Cycloparaphenylene Molecules of Various Sizes</a> Lyudmyla Adamska , Iffat Nayyar , Anna Swan , Steven Doorn , Sergei Tretiak
Friday, March 7, 2014 9:24AM - 9:36AM	<a href="#">Y2.00006: Signature of Nonadiabatic Coupling in Excited-State Vibrational Modes</a> Tammie Nelson , Miguel Soler , Adrian Roitberg , Sergei Tretiak , Sebastian Fernandez-Alberti
Friday, March 7, 2014 9:36AM - 9:48AM	<a href="#">Y2.00007: Non-Adiabatic, Multi-State Ring-Polymer Molecular Dynamics</a> Franziska Bell , Artur Menzeleev , Thomas Miller III
Friday, March 7, 2014 9:48AM - 10:00AM	<a href="#">Y2.00008: Exploring the Vibrational Stark Effect in Fullerene and Derivatives from First Principles</a> Peter Doak , Yajing Li , Douglas Natelson , Leeor Kronik , Jeffrey Neaton
Friday, March 7, 2014 10:00AM - 10:12AM	<a href="#">Y2.00009: Excitation Energy Transfer in Peridinin-Chlorophyll <math>a</math>-Protein Complex Using F<sup>o</sup> Resonance Energy Transfer</a> William Bricker , Cynthia Lo
Friday, March 7, 2014 10:12AM - 10:24AM	<a href="#">Y2.00010: Electric field manipulation of magnetoresistance in a single molecular spin-valve device</a> Kamal Dhungana , Ranjit Pati
Friday, March 7, 2014 10:24AM - 10:36AM	<a href="#">Y2.00011: Electron transfer in a two-level system within a Cole-Davidson vitreous bath</a> Mark Ratner , Mehdi Zarea , Michael Wasielewski
Friday, March 7, 2014 10:36AM - 10:48AM	<a href="#">Y2.00012: Exact factorization of the electron-nuclear wave function: General theory and applications</a> Federica Agostini , Ali Abedi , Seung Kyu Min , Yasumitsu Suzuki , E.K.U. Gross