

WEDNESDAY AFTERNOON * ROOM 28E

Natalie Stingelin, Presiding

1:30 (337). Regioregular narrow bandgap conjugated polymers for the fabrication of high performance solution deposited organic solar cells.

G.C. Bazan

2:10 (338). Soft supra-molecular nanotubes for robust light harvesting.

D.M. Eisele

2:50 (339). Size of triplet excitons in polythiophene: Evidence from resonance Raman spectra of oligomers. **M.J. Tauber**

3:10 INTERMISSION

3:30 (340). Correlating the photophysics of organic-inorganic perovskites with local chemistry. **S.D. Stranks**

4:10 (341). New ways to activate organic triplet states for photon upconversion in the visible and near-infrared. **C.J. Bardeen**, Z. Huang, X. Li, M. mabhoub, K.M. Hanson, V. Nichols, c.d. cruz, H. Le, M.L. Tang, E.L. Chronister

4:50 (342). Harvesting solar energy from singlet fission materials. A.K. Le, J. Bender, R. Pandey, A.P. Moon, **S.T. Roberts**

5:10 (343). Directional charge separation in isolated 7,8,15,16-tetraazaterrylene (TAT) crystalline nanowires. **M. Barnes**, J. Labastide, H.B. Thompson, S.R. Marques, A.L. Briseno

THURSDAY MORNING * ROOM 28E

Dmitri Kilin, Presiding

8:00 (594). Progress in solar water splitting. **B.A. Parkinson**

8:40 (595). Impact of dissociated water at photocatalytic aqueous semiconductor interfaces. **M.S. Hybertsen**

9:20 (290) Bias and energy dependent coupling between molecular states and metallic states in molecular junctions. **Z. Liu**, J. Neaton

9:40 INTERMISSION

10:05 (597). Trapping and dynamics of excess electrons at TiO₂ anatase surfaces and interfaces. **A. Selloni**

10:45 (598). Relationships between excited state dynamics and photochemistry of nanocrystal-catalyst complexes. **G. Dukovic**

11:25 (599). What makes the photocatalytic CO₂ reduction on n-doped Ta₂O₅ efficient: insights from nonadiabatic molecular dynamics. **A.V. Akimov**, R. Jinnouchi, R. Asahi, O.V. Prezhdo

THURSDAY AFTERNOON * ROOM 28E

Alexey V. Akimov, Presiding

1:30 (653). Influence of extended solvation structure upon TDDFT absorption spectra determined using intermolecular network theory and both classical and quantum mechanical treatments of nuclei. **A.E. Clark**, T. Markland, C. Isborn

2:10 (654). Nonadiabatic Excited-State Molecular Dynamics: On-the-Fly Reduction of Excited States. **T. Nelson**, S. Fernandez-Alberti, S. Tretiak

2:50 (655). Addressing the second derivative coupling in nonadiabatic molecular dynamics simulation. **G. Meek**, B.G. Levine

3:10 INTERMISSION

3:35 (656). Plexciton resonant energy transfer. **J. Yuen Zhou**

3:55 (657). Calculating non-linear properties of closed- and open-shell species with EOM-CCSD: Theory and examples. **K. Nanda**, A. Krylov

4:15 (658). Semiconductors used in photovoltaic and photocatalytic devices: Insight from DFT based calculations. **T. Le Bahers**, S. Melissen, P. Sautet, K. Takanabe

4:35 (659). Simulation of realistic electronic spectra bandshapes of chromophoric systems relevant for solar light harvesting. **M. Biczysko**, J. Bloino



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**FRONTIERS IN
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**Todd D. Krauss
Aditya Mohite
Oleg V. Prezhdo
Sergei Tretiak
Organizers**

March 13-17, 2016

San Diego Convention Center

ROOM 28E/28D/23C

SUNDAY MORNING * ROOM 28E

Valeria D. Kleiman, Presiding

8:00 Introductory Remarks.

8:05 (23). Can we really be inspired by natural light-harvesting systems to convert solar energy? Some answers from multiscale models based on quantum chemistry. **B. Mennucci**

8:45 (24). Molecular level design principles for efficient and robust light harvesting in LH2 of purple bacteria. **S. Jang**

9:25 (25). Importance of excitation and trapping conditions in photosynthetic energy transport. **R. Leon-Montiel**, I. Kassal, J.P. Torres

9:45 INTERMISSION

10:10 (26). Polynuclear Ru-based metal complexes for energy and electron transfer. L. Baraldo, **V.D. Kleiman**

10:50 (27). The effects of electronic impurities and electron-hole recombination dynamics on large grain organic-inorganic perovskite photovoltaic efficiencies. J. Blancon, W. Nie, A.J. Neukirch, G. Gupta, S. Tretiak, L. Cognet, A. Mohite, **J. Crochet**

11:30 (28). Dye-sensitized bipolar ion-exchange membranes as artificial light-driven ions pumps for use in solar fuels devices. R.S. Reiter, W. White, C.D. Sanborn, **S. Ardo**

SUNDAY AFTERNOON * ROOM 28E

Aditya Mohite, Presiding

1:30 (68). Chemistry of making and breaking of perovskites. **P.V. Kamat**

2:10 (69). Hysteresis-free large-area crystalline perovskite solar cells via temperature controlled doctor blading in ambient conditions. **G. Gupta**, A. Mallajosyula, S. Bhatt, W. Nie, A. Mohite

2:50 (70). Layered perovskite solar cells with 11.2 % efficiency, superior crystallinity and environmental stability. **H. Tsai**, W. Nie, J. Blancon, C. Stoumpos, R. Verduzco, B. Harutyunyan, S. Tretiak, G. Gupta, M.A. Alam, j. even, M.J. Bedzyk, J. Lou, P. Ajayan, M.G. Kanatzidis, A. Mohite

3:10 INTERMISSION

3:35 (71). Optoelectronic properties and molecular disorder in the plastic crystal phase of hybrid perovskites. **J. Even**

4:15 (72). Optoelectronic properties of large grain hybrid perovskites solar cells and device photo-stability. **W. Nie**

4:55 (73). Hot phonon-bottleneck in lead halide perovskite films. **Y. Yang**, M.C. Beard, J. van de Lagemaat

MONDAY MORNING * ROOM 28E

Todd Krauss, Presiding

8:00 (115). Colloidal quantum dots in extreme electromagnetic environments. **D.J. Norris**

8:40 (116). Hole transfer dynamics from QDs to tethered ferrocene derivatives. **P. Alivisatos**

9:20 (117). Bridging the gap between group IV and binary semiconducting nanocrystals: The X,L,Z motif. **N.C. Anderson**, L. Wheeler, N.R. Neale, J.S. Owen

9:40 INTERMISSION

10:05 (118). Early time carrier dynamics in quantum dot solids studied by ultrafast photocurrent spectroscopy. **V.I. Klimov**

10:45 (119). Role of surface ligands in formation of PbSe Nanoplates and their photophysics. **S.W. Kilina**

11:25 (120). Probing single-molecule interfacial electron transfer dynamics in solar energy systems. **H. Lu**

MONDAY AFTERNOON * ROOM 23C

James K. McCusker, Presiding

1:30 (153). Photocatalytic conversion of nitrobenzene to aniline through sequential proton-coupled one-electron transfers from a cadmium sulfide quantum dot. S. Jensen, S. Homan, **E. Weiss**

2:10 (154). Materials for solar energy conversion and storage. **G.A. Galli**

2:50 (155). Spin resolved electron dynamics of vanadium (IV) doped anatase. S.J. Jensen, T.M. Inerbaev, **D. Kilin**

3:10 INTERMISSION

3:30 (156). Ultrafast charge transfer-state dynamics in first-row transition metal-based complexes: Making earth-abundant chromophores viable for light harvesting applications. **J.K. McCusker**

4:10 (157). Electronic processes in low bandgap polymers for OPV and photocatalytic applications. **L.X. Chen**

4:50 (158). Effects of charge delocalization on long-lived charge carriers in low dielectric media. **G. Rumbles**

TUESDAY MORNING * ROOM 28D

Oleg V. Prezhdo, Presiding

8:00 (217). Charge separation and recombination at single-walled carbon nanotube photovoltaic interfaces. **J. Blackburn**, A. Ferguson, O. Reid, R. Ihly, A. Dowgiallo, S.L. Guillot, P. Schulz, M. Yang, K. Zhu, J. Berry, K. Mistry, N. Kopidakis, G. Rumbles

8:40 (218). Exciton transport in thin films of semiconducting carbon nanotubes using 2D white-light spectroscopy. **M.T. Zanni**, M. Arnold

9:20 (219). Design of better photovoltaic materials with cheminformatics approaches. **O. Isayev**

9:40 INTERMISSION

10:05 (220). Insight into carbon nanotube surface structures for photovoltaics applications. **S.K. Doorn**, N. Hartmann, N. Subbaiyan, R. Pramanik, A. Mallajosyula, A. Mohite, J. Blackburn

10:45 (221). Interplay between singlet fission and triplet transport in organic semiconductors revealed by ultrafast microscopy. T. Zhu, Y. Wan, Z. Guo, J.C. Johnson, **L. Huang**

11:25 (222). Self-assembled molecular p/n junctions for application in dye-sensitized solar energy conversion. **B.H. Farnum**, K. Wee, T.J. Mey

WEDNESDAY MORNING * ROOM 28E

Sergei Tretiak, Presiding

8:00 (285). Artificial photosynthesis: Progress, science prospects and technology outlook. **H. Atwater**

8:40 (286). Effect of intra- and interchain interaction on energy transfer in single conjugated polymers and aggregates. **D. Vanden Bout**, Z. Hu

9:20 (287). Evolutionary design of emitters for organic light-emitting diodes. **Y. Shu**, B.G. Levine

9:40 INTERMISSION

10:05 (288). On the role of intermixed phases in organic photovoltaic blends. **N. Stingelin**

10:45 (289). Entropy and disorder enable charge separation in organic solar cells. S. Hood, **I. Kassal**

11:25 (290). (596). Efficient computational screening tool for Ru(II) light harvesters. **L.A. Fredin**, T.C. Allison