

# Informed Design of Quantum Dots and Quantum Dot Assemblies for Energy Applications

Organizers: Stephanie Brock, Zhenfei Liu, Jier Huang

New Orleans, LA

March 18-19, 2024

## Monday, March 18, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R07

A. Chakraborty, Z. Liu, *Presiding*

**8:00 AM.** Introductory Remarks.

**8:10 AM.** Designing quantum dots for photocatalytic, optoelectronic and photonic applications. **D. Ma**

**8:35 AM.** Improving photon upconversion and photoluminescence via triplet transfer from photoexcited nanocrystals. **M.L. Tang**

**9:00 AM.** Theory of conical intersections as a tool for nanoscience. **B.G. Levine**, M. Esch, C. Hetherington, F. Liang, A. Mehmood, W. Peng, Y. Shu

**9:20 AM.** Tuning electronic coupling in silicon quantum dot-molecular hybrid systems via the binding bridge for photon upconversion. **K. Wang**, N.Q. Nguyen, M.L. Tang, T.A. Su

**9:35 AM.** Vibronic coherence in photoinduced charge transfer in CdSe quantum dots. **W.F. Beck**, N. Mohan T. M.

**10:00 AM.** Intermission.

**10:20 AM.** Understanding covalency and magnetism in Ln<sup>3+</sup> doped CrI<sub>3</sub>. **X. Li**

**10:45 AM.** Investigation of radiative and non-radiative electron-hole recombination rates in semiconductor nanoparticles using kinetic Monte Carlo method. C. Martin, N. Spanedda, J. Beyer, **A. Chakraborty**

**11:05 AM.** Acetylene spacers between CdSe QDs and anthracene: The effect of driving force and reorganization energy on triplet energy transfer. **T. Miyashita**, S. He, P. James, A. Kaledin, J. Merham, D. Fishman, T. Lian, M.L. Tang

**11:20 AM.** Taking inspiration from molecular photochemistry for quantum dots: Hot carrier cooling via a cascade of conical intersections. **C.V. Hetherington**, B.G. Levine

## Monday, March 18, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R07

S. L. Brock, L. Luo, *Presiding*

**2:00 PM.** Driving multielectron redox catalysis with photoexcited nanocrystals. **G. Dukovic**

**2:25 PM.** A nano-biological living system for the production of solar fuels. E. Edwards, J. Jelusic, R.M. Kosko, K. McClelland, S. Ngarnim, W. Chiang, S. Lampa-Pastirk, K. Bren, **T.D. Krauss**

**2:45 PM.** Photocatalytic CO<sub>2</sub> reduction employing quantum dot light absorbers: Elucidating underlying charge transfer mechanisms. **J.H. Olshansky**

**3:05 PM.** Silicon nanocrystal hybrid photocatalysts for CO<sub>2</sub> reduction. **N.R. Neale**

**3:30 PM.** Metal chalcogenide quantum dot gel as a unique photocatalyst for organic synthesis. **L. Luo**, D. Liu, A. Hazra, R. Maity

**3:55 PM.** Intermission.

**4:15 PM.** Designing effective quantum dot photocatalytic systems for green hydrogen production. **L. Amirav**

**4:40 PM.** CdS quantum dot assemblies for photocatalytic water reduction: Aggregation vs oxidative assembly. **V. Alevato**, D. Streater, C. Premtaj, J. Huang, S.L. Brock

**4:55 PM.** Quantum size confinement effect controls photocatalytic H<sub>2</sub> evolution and photovoltage in CdSe nanocrystals. **F.E. Osterloh**

**5:20 PM.** CdS quantum dot gel as a direct hydrogen-atom transfer photocatalyst for C(sp<sup>3</sup>)-H functionalization. **D. Liu**, A. Hazra, L. Luo

**5:35 PM.** Spin trapping: A tool for observing reactions at metal chalcogenide quantum dot surfaces. C.J. Aschendorf, K.V. Prather, M. Degbevi, **E.Y. Tsui**

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J. R. Caram, K. E. Shulenberger, *Presiding*

**8:00 AM.** First principle studies of semiconducting nanoparticles and nanoplatelets for electronic and solar energy devices. **G.A. Galli**

**8:25 AM.** Controlling opto-electronic properties of QD arrays through beneficial ligand/QD interactions. **M.C. Beard**

**8:50 AM.** Quantitative comparison of recombination rates of core/shell quantum dots in colloidal solutions and self-assembled monolayer superlattices. **R.M. Brinn**, C. Yan, J. Ondry, A.S. Abbas, P. Alivisatos

**9:05 AM.** Film photon correlation methods: Extracting single nanocrystal properties from device-relevant films. **K.E. Shulenberger**

**9:25 AM.** Photo-induced reversible ligand detachment from CdSe quantum dots. M.N. Grega, J. Gan, M. Noman, **J. Asbury**

**9:50 AM.** intermission.

**10:10 AM.** Surface chemistry tunes electronic and optical properties of plasmonic metal oxide nanocrystals. **D.J. Milliron**

**10:35 AM.** Understanding the ligand exchange in CdS quantum dots from first principles. **J. Frimpong**, S. Aryal, Z. Liu

**10:50 AM.** Colloidal quantum shells: An emerging 2D morphology for energy applications. **M. Zamkov**

**11:15 AM.** Mesoscale colloidal nanoplatelets for direct device integration. **J.R. Caram**

**11:35 AM.** Harnessing sequence-defined polymers for the dynamic assembly of colloidal quantum dots. **B.M. Cossairt**, C. Lowe, H. Larson, E. Miura-Stempel

## Tuesday, March 19, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R07

J. Huang, R. D. Schaller, *Presiding*

**2:00 PM.** Design of semiconductor nanomaterials with cognizance of lattice dynamics. **R.D. Schaller**

**2:25 PM.** Coherent electron transfer in quantum dot molecules. **E. Rabani**

**2:45 PM.** Tracking energy transfer pathways in halide perovskite-rhodamine dye assemblies. A. Chemmangat, J. Chakkamalayath, J. DuBose, **P.V. Kamat**

**3:10 PM.** Long-wavelength continuum model for molecular excitonic systems. **C. Chuang**, J. Cao

**3:30 PM.** The role of interfacial structure in modifying electronic excitations in nanomaterials. **A.M. Rappe**

**3:55 PM.** Intermission.

**4:15 PM.** Ab initio excited state dynamics in quantum dots: Semiconducting, metallic and perovskites. **O.V. Prezhdo**

**4:40 PM.** Resolving the excited state dynamics of  $\text{In}_x\text{Ga}_{1-x}\text{P}$  QDs. **B.C. Li**, A. Gupta, S. Sohoni, P. Wu, J. Ondry, R.D. Schaller, D. Talapin, G.S. Engel

**4:55 PM.** Tuning the biradical character of graphene quantum dots by insertion of *h*-BN domains. **H. Lischka**, A. Aquino, L. dos Santos, F. Machado

**5:15 PM.** Comparing atomic lattice resolved electron tomography in multiple different 3D self-assembled PbSe superlattice mesocrystals. E. Field, G. Kim, M. Law, **A.J. Moule**

**5:35 PM.** Light driven  $\text{H}_2$  generation in Pt-tipped CdS nanorods: Dependence on the Pt size and CdS rod length. **T. Lian**

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