EFRC: CENTER FOR ADVANCED SOLAR PHOTOPHYSICS (CASP)

UPDATED: AUGUST 2016

AWARDS: $19.0M (August 2009 – July 2014); $11.2M (August 2014 – July 2018)
WEBSITES: http://science.energy.gov/bes/efrc/centers/casp/; http://casp.lanl.gov
TEAM: **Los Alamos National Laboratory (Lead):** Victor Klimov (Director), Jeff Pietryga, István Robel, Kirill Velizhanin; **National Renewable Energy Laboratory**: Matt Beard (Associate Director), Justin Johnson, Joey Luther, Art Nozik; **University of California, Irvine**: Matt Law; **University of Minnesota**: Uwe Kortshagen; **George Mason University**: Alexander Efros, Andrew Shabaev; **University of Pennsylvania**: Cherie Kagan; **University of Chicago**: Giulia Galli

SCIENTIFIC MISSION AND APPROACH

CASP's mission is to investigate and harness the interactions between nanomaterials and light to produce fundamental breakthroughs that will enable the next generation of low-cost, high-efficiency solar energy conversion systems. CASP's focus is on solution-processible semiconductor nanocrystals, or quantum dots (QDs), that are small enough to exhibit "quantum confinement," a phenomenon which affects the interactions of these structures with light and each other in profound ways. QD properties can be tailored by varying particle composition, size, shape, internal structure, and inter-particle interactions. CASP is organized into three thrusts:

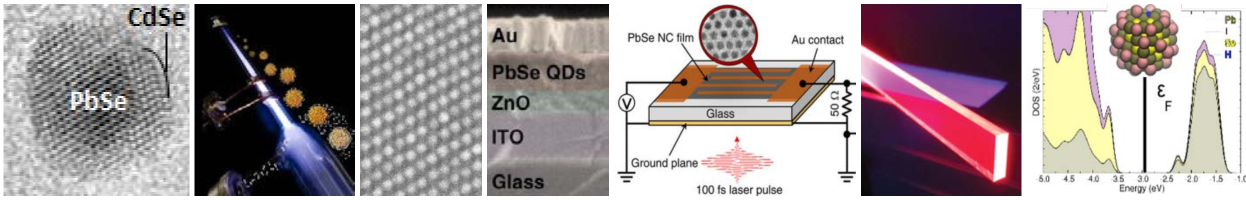
Novel Physical Phenomena: Combines capabilities in optical and scanning-probe spectroscopies emphasizing state-of-the-art femtosecond and single-dot techniques with theory, modeling and simulation including effective-mass, tight-binding, quantum chemistry, and atomistic approaches.

Novel NanoMaterials: Provides advanced capabilities for implementing materials-by-design concepts in the synthesis of engineered nanocrystals and multifunctional nanocomposites using colloidal and plasma-based techniques.

Charge Manipulation and Exploratory Devices: Houses unique capabilities for probing charge transport in mesoscopic QD arrays, as well as for fabrication and characterization of QD-based energy conversion architectures that exploit novel nanoscale physics.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Demonstrated enhanced carrier multiplication (CM) within quantum-confined nanocrystals that allows for the conversion of single high-energy photons into multiple electron-hole pairs and the development of rigorous experimental protocols for quantifying CM efficiencies.
- Demonstrated record-high CM yields in engineered core/shell QDs via suppression of the "cooling" of highly-excited (or "hot") charge carriers, which competes with multiexciton generation. Foundational stability and charge transport studies of QD films resulted in the demonstration of record-high carrier mobilities via intelligent control of QD surfaces and inter-particle coupling.
- Demonstrated the first stable QD-based solar cells with certified power conversion efficiencies, establishing a new technology class ("quantum-dot solar cells") on the official PV efficiency chart.
- Made the first solar cell with quantum efficiency greater than 100%, breaking the Shockley-Queisser limit, and confirming that CM enhances the performance of real-life QD-based photovoltaic devices.
- Synthesized a variety of novel engineered nanocrystals, including advanced nanoheterostructures and doped, alloyed, and ligand-free Group IV QDs.
- Developed the underlying principles of QD-based luminescent solar concentrators, and demonstrated efficient devices with dimensions relevant to use as "solar windows."



CASP research, from left: Heterostructured QDs by colloidal synthesis exhibit tunable optical properties; Plasma synthesis allows Group IV QDs with tunable composition and size; Solution-cast QD films can be highly ordered; PbSe QD solar cells offer extra current via CM; Transient photoconductivity allows for monitoring charge-carrier dynamics in QD films in real time; Luminescent solar concentrators for "solar windows"; Density functional theory connects optical and electronic properties of QDs to the structure of their interior and surfaces.

IMPACT

- CASP has supported and organized multiple international conferences devoted to QD research, including the "7th International Conference on Quantum Dots" (2012), and "20 Years of Quantum Dots at Los Alamos" (2015). CASP has also supported and organized energy- and nanomaterial-focused symposia at national meetings for major scientific societies, including the APS (2015, 2016), MRS (2015, 2011), ACS (2012, 2011), AVS (2011), and AIChE (2011).
- The CASP YIC organizes the biennial "CASP Summer School". This two-day event is held at a CASP partner site, and brings together an impressive lineup of world leaders in QD and solar energy research for a mixture of topical seminars and direct discussions with local scientists and students.
- **UbiQD, LLC**, is a technology company based in Los Alamos, NM, dedicated to the manufacturing and applications development for luminescent QDs based on non-toxic metals, including copper indium sulfide QDs originally developed for QD-sensitized solar cells within CASP. The company was founded in 2014 by Dr. Hunter McDaniel, former chair of the CASP Young Investigator's Committee (YIC); a joint CASP-UbiQD publication appeared in *Nature Nanotechnology* in 2015. http://www.ubiqd.com

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of May 2016, CASP had published 146 peer-reviewed publications cited over 10,000 times and filed 6 patent disclosures and 5 US patent applications; 2 patents have been issued. The following is a selection of impactful papers:

- Crisp, R. W., *et al.* Metal halide solid-state surface treatment for high efficiency PbS and PbSe QD solar cells. *Sci. Reports.* **5**, 9945, doi: 10.1038/srep09945 (2015). [**36 citations**]
- Zhang, J., *et al.* PbSe quantum dot solar cells with more than 6% efficiency fabricated in ambient atmosphere *Nano Lett.* **14**, 6010-6015, doi: 10.1021/nl503085v (2014) [**47 citations**]
- Meinardi, F., *et al.* Large-area luminescent solar concentrators based on 'Stokes-shift-engineered' nanocrystals in a mass-polymerized PMMA matrix. *Nat. Photon.* **8**, 392-399, doi: 10.1038/nphoton.2014.54 (2014). [**119 citations**]
- Wheeler, L. M., *et al.* Hypervalent surface interactions for colloidal stability and doping of silicon nanocrystals. *Nat. Commun*. **4**, 2197, doi: 10.1038/ncomms3197 (2013). [**47 citations**]
- McDaniel, H., *et al.* An integrated approach to realizing high-performance liquid-junction quantum dot sensitized solar cells. *Nat. Commun.* **4**, 2887, doi: 10.1038/ncomms3887 (2013). [**79 citations**]
- Semonin, O. E., *et al.* Peak external photocurrent quantum efficiency exceeding 100% via MEG in a quantum dot solar cell. *Science* **334,** 1530-1533, doi:10.1126/science.1209845 (2011). [**646 citations**]
- Galland, C., *et al.* Two types of luminescence blinking revealed by spectroelectrochemistry of single quantum dots. *Nature* **479**, 203-207, doi: 10.1038/nature10569 (2011). [**299 citations**]
- Liu, Y., *et al.* Dependence of carrier mobility on nanocrystal size and ligand length in PbSe nanocrystal solids. *Nano Lett.* **10**, 1960-1969, doi:10.1021/nl101284k (2010). [**313 citations**]
- Luther, J. M., *et al.* Stability assessment on a 3% bilayer PbS/ZnO quantum dot heterojunction solar cell. *Adv. Mater.* **22**, 3704-3707, doi**:** 10.1002/adma.201001148 (2010). [**208 citations**]