Center for Advanced Solar Photophysics (CASP)
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Lead Institution: Los Alamos National Laboratory
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Mission Statement*: To exploit fundamental interactions between nanomaterials and light with the goal of producing disruptive advances in the efficiency of solar energy conversion.*

Solar light is a tremendous resource of clean energy. Widespread use of solar energy will require technologies that offer a dramatic increase in photoconversion efficiency *simultaneously* with reduced cost, which will require disruptive advances relying on new physical principles and novel materials. Quantum-confined semiconductor nanocrystals (NCs) are fascinating structures offering tremendous promise in the area of solar energy conversion into either electricity or chemical fuels. The development of NC-based approaches lies at the intersection of chemistry, physics, materials science and engineering. The Center for Advanced Solar Photophysics (CASP) unites world-class experts spanning these disciplines toward the purpose of harnessing the unique properties of quantum-confined semiconductor materials to facilitate the realization of the next generation of low-cost, high-efficiency solar photoconversion systems.

As an established leader in the design, synthesis and exploitation of novel nanomaterials that exhibit advanced, solar-relevant physical phenomena, CASP continually strives to achieve new levels of efficiency in NC-based photovoltaic (PV) devices. In addition, we are vigorously investigating a broad range of approaches toward applying the unique properties of nanomaterials to boost the efficiencies of existing or emerging PVs above present limits. This multifaceted research program is captured in four main Themes (Fig. 1), each of which strives to address a specific, essential question:

- *How can we enhance the efficiency of carrier multiplication in engineered nanomaterials?* The observation of carrier multiplication (the generation of multiple excitons by a single absorbed photon) in NC-based PVs is a singular example of advanced nanoscale physics being brought to bear on real solar cells. While the efficiencies of this phenomenon in NCs are enhanced relative to those in bulk semiconductors, they are still not high enough to considerably impact power conversion efficiency limits. In the **Carrier Multiplication by Design Theme**, we investigate how structure-based control over carrier cooling, and carrier-photon and carrier-carrier interactions can drive CM efficiency to the theoretical limit.
- *How can we use nanomaterials to harness the full solar spectrum more efficiently?* The ultimate conversion efficiency of standard PV devices is limited by two main channels of energy loss: the inability to capture lower-energy, sub-band-gap photons, and the dissipation of the excess energy of above-band-gap photons as heat. In the **Advanced Photon Management Theme**, we employ NCs to make better use of such photons through up- or down-conversion schemes (collectively called “spectral reshaping”) as well as to augment sunlight harvesting with inexpensive luminescent solar concentrators.
- *How can we manipulate inter-particle coupling to control charge and energy transport in mesoscopic assemblies?* Our understanding of the unique physical phenomena that arise in nanoscale materials has rapidly advanced, but to be relevant, these phenomena must be active in macroscopic devices. In the **Functional Mesoscopic Assemblies Theme**, we develop approaches for integrating engineered NCs into mesoscopic assemblies that retain original functionalities and augment them with efficient carrier transport and other emergent phenomena associated with controlled inter-particle coupling.

- *How can unique nanoscale phenomena be exploited in advanced photoconversion devices?* Currently, optimizing the performance of solar cells based on NCs relies on tuning their properties to meet the needs of a conventional PV architecture. To overcome the limitations of this traditional concept, in the **Advanced Device Architectures Theme**, we will explore new photoconversion schemes tailored for a specific nanostructure and optimized *via* convergent evolution of both the material and the device architecture.

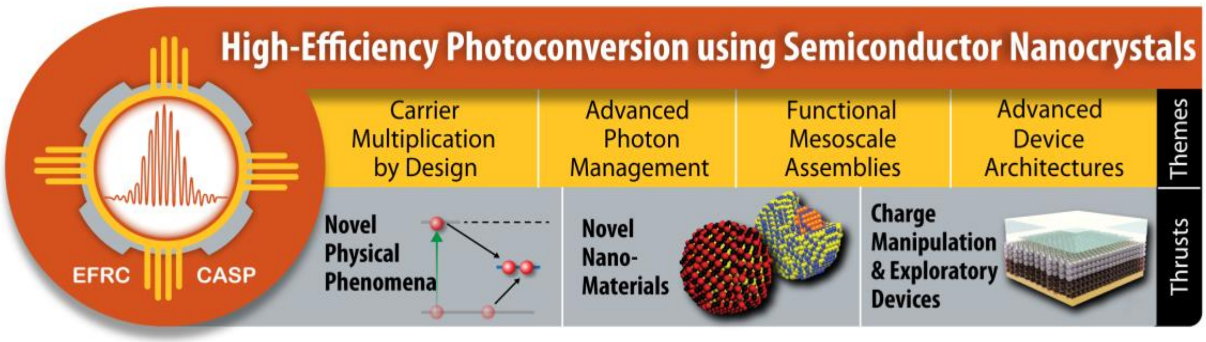

Figure 1. Research themes address essential questions using the capabilities housed within CASP's three Thrusts.

To tackle these research Themes we utilize world-class capabilities and expertise organized within a Thrust structure that supports a comprehensive approach to all relevant aspects of each problem. The **Novel Physical Phenomena (NPP) Thrust** combines capabilities in optical and scanning-probe spectroscopies emphasizing state-of-the-art femtosecond and single-NC techniques with theory, modeling and simulation that encompass effective-mass, tight-binding, quantum chemistry, and atomistic techniques. The **Novel NanoMaterials (NNM) Thrust** provides advanced capabilities for implementing materials-by-design concepts in the synthesis of engineered NCs and multifunctional nanocomposites using colloidal and plasma-based techniques. Finally, the **Charge Manipulation and Exploratory Devices (CMD) Thrust** houses unique capabilities for probing transport in mesoscopic QD arrays, as well as for fabrication and characterization of NC-based devices with architectures that exploit novel nanoscale physics.

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