Approaches to Future Generation Photovoltaics and Solar Fuels: *Multiple Exciton Generation in Quantum Dots, Quantum Dot Arrays, Molecular Singlet Fission, and Quantum Dot Solar Cells*

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Abstract

One potential, long-term approach to more efficient future generation solar cells for solar electricity and solar fuels is to utilize the unique properties of quantum dots (QDs) and unique molecular chromophores to control the relaxation pathways of excited states to produce enhanced conversion efficiency through efficient multiple electron-hole pair generation from single photons . We have observed efficient multiple exciton generation (MEG) in PbSe, PbS, PbTe, and Si QDs and efficient singlet fission (SF) in molecules that satisfy specific requirements for their excited state energy level structure to achieve carrier multiplication. We have studied MEG in close-packed QD arrays where the QDs are electronically coupled in the films and thus exhibit good transport while still maintaining quantization and MEG. We have developed simple, all-inorganic solution-processable QD solar cells that produce large short-circuit photocurrents and power conversion efficiencies above 5% via both nanocrystalline Schottky junctions and nanocrystalline p-n junctions. These solar cells also show QYs for photocurrent that exceed 100% in the photon energy regions where MEG is possible; the photocurrent MEG QYs as a function of photon energy match those determined via time-resolved spectroscopy. We have also observed very efficient SF in thin films of molecular crystals of 1,3 diphenylisobenzofuran with quantum yields of 200% at the optimum SF threshold of 2Eg (HOMO-LUMO for S_0-S_1)), reflecting the creation of two excited triplet states from the first excited singlet state. Various possible configurations for novel solar cells based on MEG in QDs and SF in molecules that could produce high conversion efficiencies will be presented, along with progress in developing such new types of solar cells. Recent analyses of the effect of MEG or SF combined with solar concentration on the conversion efficiency of solar cells will also be discussed.