

MOLECULE-LIKE CdSe NANOCCLUSERS PASSIVATED WITH STRONGLY INTERACTING LIGANDS: ENERGY LEVEL ALIGNMENT AND PHOTOINDUCED ULTRAFAST CHARGE TRANSFER PROCESSES

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Semiconductor nanoclusters (SCNCs) are promising electronic materials for use in solid-state device fabrication, where device efficiency is strongly controlled by charge generation and transfer from SCNCs to their surroundings. In this paper we report the excited-state dynamics of molecule-like 1.6 nm diameter CdSe SCNCs, which are passivated with the highly conjugated ligand phenyldithiocarbamate (PDTC) or para-substituted PDTCs. Femtosecond transient absorption studies reveal sub-picosecond hole transfer ($\tau \approx 0.9$ ps) from a SCNC to its ligand shell based on strong electronic interaction and hole delocalization, and hot electron transfer ($\tau \approx 0.2$ ps) to interfacial states created by charge separation. A series of control experiments were performed by varying SCNC size (1.6 nm v.s. 2.9 nm) and photon energy of the pump laser (388 nm v.s. 490 nm), as well as addition of electron quencher (benzoquinone) and hole quencher (pyridine), which rules out alternative mechanisms and confirms the critical role of energy level alignment between the SCNC and its passivating ligands.

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