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Electronic and Optical Properties of Core/Shell $Pb_{16}X_{16}/Cd_{52}X_{52}$ (X=S, Se, Te) Quantum Dots PATRICK TAMUKONG, North Dakota State University, MICHAEL MAYO, Retired, SVETLANA KILINA, North Dakota State University — The electronic and optoelectronic properties of semiconductor quantum dots (QDs) are mediated by surface defects due to the presence of dangling bonds producing trap states within the HOMO-LUMO energy gap, and contributing to fluorescence quenching. Surface capping ligands are generally used to alleviate this problem and increase the quantum yields of QDs. An alternative way is to synthesize core-shell QD structures; i.e., a QD core with a shell of another semiconductor material. We have investigated the effects of $Cd_{52}X_{52}$ shells on the photoexcited dynamics of $Pb_{16}X_{16}$ (X=S, Se, Te) QDs. The thin (≈ 0.50 nm) shells were found to result largely in type I core/shell structures and a blue shift of the absorption spectra. Our studies revealed fairly strong core-shell hybridization in the electronic states close to the conduction band (CB) edge for $Pb_{16}S_{16}$ and $Pb_{16}Se_{16}$ cores, whereas for the $Pb_{16}Te_{16}$ core, such CB states were largely shell-like in nature. Nonadiabatic DFT-based dynamics, coupled with the surface hopping method, was used to study the effects of the core and shell compositions on energy relaxation rates in these systems.

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