Controlling relaxation rates of electron/hole pair by chemical composition of $(PbX)_{16}/(CdX)_{52}$, (X = S, Se) core/shell quantum dots

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Colloidal quantum dots (QDs) can be made to be suitable for many areas of science. The ability of QDs to be used in a wide range of application is in part due to the manipulation of the QDs' surface or composition. Traditionally, the ligands coordinated to the surface of the QDs were used to tailor the QDs to the particular application. However, the coordination of the ligands are dynamic and can cause lose in adventitious properties. Alternatively, the surface of the QDs can be covered by a large band gap material which can isolate the core from the environment. This shell can also be used to manipulate the electronic and thereby manipulate the photoexcitation dynamic properties. This study investigates the effect of chemical composition on the relaxation rates of the electron/hole pair in $(PbX)_{16}/(CdX)_{52}$, (X = S, Se) core/shell. The ground state electronic properties of the two systems have similar features for optical excitation, surface morphology and electron density. However, the non-adiabatic coupling terms for $(PbS)_{16}/(CdS)_{52}$ are nearly twice larger compared to $(PbSe)_{16}/(CdSe)_{52}$, leading to longer lived hot electron/hole pairs in $(PbSe)_{16}/(CdSe)_{52}$. The longer lived hot electron/hole pair in $(PbSe)_{16}/(CdSe)_{52}$ could allow for multi-exciton generation to be more favorable compared to $(PbS)_{16}/(CdS)_{52}$. Unfortunately, the electron and hole relax to the core of the core/shell QD. Additional research is needed to fully realize the full potential of the core/shell QDs in solar cell application.