

Abstract Submitted
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Excitons and band edge alignment in CdSe/CdS core-shell nanocrystals: ab initio DANYLO ZHEREBETSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, COMPUTATIONAL MATERIALS SCIENCE AND NANOSCIENCE TEAM — Quantum confinement is a foundational nanoscience concept that allows tuning electronic properties of quantum dots. Core-shell quantum dots are promising nanoparticles and found applications as light-emitting optoelectronic devices and biomarkers [1] due to their robustness and tunability of both core and shell. The fluorescent quantum yield of these quantum dots can achieve 100% [2] even at room temperature [3]. However, to understand many phenomena of carrier dynamics, photoluminescence efficient and Auger effects, fine electronic structures of the exciton are needed. Here, using large scale electronic structure calculations based on charge patching method, we have investigated the exciton binding energy, band alignment between core and shell, charge separation between electron and hole. We will discuss how these can be tuned by changing the core/shell dimensions. 1. Shirasaki Y., Supran G., Bawendi M., Bulović V. *Nature Photonics* 7, 13 (2013). 2. Javaux C. et al, *Nature Nanotech.* 8, 206 (2013) 3. Achieved in Alivisatos lab (2014).

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