Electronic Structure of PbSe/PbS Core-Shell Quantum Dots

ADAM BARTNIK, Cornell University, EFRAT LIFSHITZ, Israel Institute of Technology, FRANK WISE, Cornell University — The electronic structure of PbSe/PbS core-shell Quantum Dots (QDs) is calculated within a 4-band envelope function theory and compared to experimentally observed absorption spectra [1]. Our theory extends the isotropic effective mass approximation used successfully in PbS and PbSe core QDs [2] to be valid across discontinuous barriers in material parameters. Even though the band gaps of PbSe and PbS present a Type-II heterostructure, the model predicts that at typical QD sizes, these Type-II effects will not be seen. In fact, the wavefunctions are predicted to extend evenly over both materials except in the largest of sizes. This unusual lack of confinement is explained, and is shown to agree well with recent experimental results. [1] E. Lifshitz, et. al. Air-stable PbSe/PbS and PbSe/PbSe_{x}S_{1-x} core-shell nanocrystal quantum dots and their applications. Journal of Physical Chemistry B, 2006. [2] I. Kang and F. W. Wise. Electronic structure and optical properties of PbS and PbSe quantum dots. J. Opt. Soc. Am. B, 14(7):1632, July 1997.

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