Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

The Peculiar electronic structure of PbSe quantum dots[1] JOONHEE AN, ALBERTO FRANCESCHETTI, S. DUDIY, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401 — PbSe quantum dots have recently emerged as promising systems that may realize direct carrier multiplication (DCM) for solar cell applications. We have calculated the underlying electronic/optical structure of PbSe nanocrystals with an atomistic pseudopotential method, finding that the electronic structure is more subtle than k·p or tight-binding calculations have previously suggested. The following two effects emerge from our calculations: (i) The bulk-degenerate L states forming the VBM and CBM are split due to (1) valley-valley coupling, (2) valence-conduction interband coupling, and (3) the strong anisotropy of the bulk L valleys. Optical absorption is dictated by transitions among anisotropic dot states characteristic of transverse and longitudinal effective masses. Our calculated optical absorption spectrum is in good agreement with experiment. In particular, our calculation reproduces the measured second absorption peak that had previously been attributed to forbidden transitions $1S_h \rightarrow 1P_e$ or $1P_h \rightarrow 1S_e$ on the basis of k·p and tight-binding calculations. (ii) Using our calculated single-particle states, we evaluate DCM mechanism, showing that the rate of X-to-XX (exciton to biexciton) transitions far exceeds the reverse, XX-to-X rate, thus opening the way to efficient DCM.

[1]Supported by DOE-SC-BES-DMS under NREL contract No. DE-AC36-99GO10337

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Date submitted: 28 Nov 2005 Electronic form version 1.4