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Carrier Multiplication in Semiconductor Nanocrystals: Theoretical Screening of Candidate Materials JUN-WEI LUO, ALBERTO FRANCESCHETTI, ALEX ZUNGER, National Renewable Energy Lab — The process of Direct Carrier Multiplication (DCM) involves the creation of TWO electron-hole pairs as a results of exciting a nanostructure by ONE photon with energy two times larger than the band gap E_g. The ratio $R(E) = \rho_{XX}(E)/\rho_X(E)$ between the biexciton (XX) and monoexciton (X) density of states [Nano Lett. **6**, 2191 (2006)] is a "figure of merit" of the DCM process. Using the "Truncated Crystal" approximation to the electronic structure of nanocrystals based on the atomistic, semi-empirical pseudopotential approach we calculated $R(E)$ for nanocrystals of GaSb, InAs, InP, GaSb, InSb, Ge, Si, and PbSe. We found that InSb, GaSb, Ge, and PbSe quantum dots have larger DCM figure of merit than the other quantum dots. Our calculations suggest that there are three requirements for high DCM efficiency: (1) Small nanocrystal band gap (< 1.6 eV) to match the solar spectrum, (2) high degeneracy of the band-edge states, and (3) heavy electron and hole effective mass. We conclude that nanocrystal made of HgS, HgTe, HgSe, PbS, PbTe, and Sn are also good candidates for DCM-based solar cells.

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