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Influence of the electronic structure and the multi-exciton spectral density on the multiple exciton generation in semiconductor nanocrystals CHRISTOPHE DELERUE, IEMN-ISEN, Lille, France, GUY ALLAN, IEMN-ISEN — Several experimental works have reported that a single high-energy photon could generate multiple excitons in semiconductor nanocrystals and several theories are proposed to explain these results. We calculate the electronic structure of InAs, Si and PbSe nanocrystals and we investigate two models of the multiple exciton generation (MEG). We show that the impact ionization process is efficient at high energy, with lifetimes as small as 10 fs. We present simulations of the MEG showing that, in PbSe and Si nanocrystals, the impact ionization alone cannot explain the observed efficiencies, even without relaxation by electron-phonon scattering. We calculate the spectral densities of multi-exciton states and we evaluate the possibility of direct photo-generation of multi-excitons. We confirm the importance of the multi-exciton spectral densities because of their rapid variation over several orders of magnitude. The high MEG efficiencies in PbSe and Si nanocrystals imply a very efficient relaxation in multi-exciton states characterized by a negligible density.

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