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Enhanced Multiple Exciton Generation in Amorphous Silicon Nanoparticles[1] ANDREI KRYJEVSKI, DEYAN MIHAYLOV, North Dakota State Univ, DMITRI KILIN, University of South Dakota — Multiple exciton generation (MEG) in nm-sized hydrogen-passivated silicon nanowires (NWs), and quasi two-dimensional nanofilms depends strongly on the degree of the core structural disorder as shown by the many-body perturbation theory (MBPT) calculations based on the DFT simulations. Here, we use the HSE exchange correlation functional. In MBPT, we work to the 2nd order in the electron-photon coupling and in the approximate screened Coulomb interaction. We also include the effect of excitons for which we solve Bethe-Salpeter Equation. We calculate quantum efficiency (QE), the average number of excitons created by a single absorbed photon, in 3D arrays of $Si_{29}H_{36}$ quantum dots, NWs, and quasi 2D silicon nanofilms, all with both crystalline and amorphous core structures. Efficient MEG with QE of 1.3 up to 1.8 at the photon energy of about $3E_g$, where E_g is the gap, is predicted in these nanoparticles except for the crystalline NW and film where QE $\simeq$ 1. MEG in the amorphous nanoparticles is enhanced by the electron localization due to structural disorder. The exciton effects significantly red-shift QE(E_{photon}) curves. Nanometer-sized amorphous silicon NWs and films are predicted to have effective MEG within the solar spectrum range.

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