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Multiple Exciton Generation in Semiconductor Nanostructures: DFT-based Computation DEYAN MIHAYLOV, ANDREI KRYJEVSKI, DMITRI KILIN, SVETLANA KILINA, North Dakota State Univ, DAYTON VOGEL, University of South Dakota — Multiple exciton generation (MEG) in nm-sized H-passivated Si nanowires (NWs), and quasi 2D nanofilms depends strongly on the degree of the core structural disorder as shown by the perturbation theory calculations based on the DFT simulations. In perturbation theory, we work to the 2^{nd} order in the electron-photon coupling and in the (approximate) RPA-screened Coulomb interaction. We also include the effect of excitons for which we solve Bethe-Salpeter Equation. To describe MEG we calculate exciton-to-biexciton as well as biexciton-to-exciton rates and quantum efficiency (QE). We consider 3D arrays of Si29H36 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 $3E_{gap}$ 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 vs. photon energy curves. Nm-sized a-Si NWs and films are predicted to have effective MEG within the solar spectrum range. Also, we find efficient MEG in the chiral single-wall Carbon nanotubes and in a perovskite nanostructure.

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