Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Carrier Multiplication in Chiral Single-Walled Carbon Nanotubes: DFT-Based Study. DEYAN MIHAYLOV, ANDREI KRYJEVSKI, SVETLANA KILINA, DMITRI KILIN, North Dakota State University — It is understood that the conclusion about multiple exciton generation (MEG) efficiency in a nanoparticle can only be made by including competition between different relaxation channels, such as phonon-mediated carrier thermalization, exciton multiplication and recombination, Auger scattering, etc. Here, we study time evolution of photo-excited states using Boltzmann transport equation (BE) that includes phonon emission/absorption terms together with the exciton multiplication and recombination terms. BE coefficients are computed using finite-temperature many-body perturbation theory (MBPT) (sometimes called NEGF) combined with the DFT simulations. Exciton effects are included by solving the Bethe-Salpeter equation based on RPA-screened Coulomb interaction (with additional simplifying approximations). In particular, we calculate internal efficiency, the number of excitons generated from a single energetic photon. We find that efficient MEG in chiral single-wall carbon nanotubes (SWCNTs), such as (6,2), (10,5), (6,5), and in nm-sized amorphous H-passivated Si nano-wires is present within the solar spectrum range. In SWCNTs MEG strength depends on chirality. We find that MEG efficiency in SWCNTs with Cl atoms adsorbed to the surface is enhanced compared to the pristine case.

Deyan Mihaylov
North Dakota State University

Date submitted: 11 Nov 2016 Electronic form version 1.4