Non-radiative relaxation dynamics of photo-induced excitons in (5,0) carbon nanotube and semiconducting PbSe nanowire interface

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Photo-induced creation of excitons are explored, and subsequently the non-radiative relaxation dynamics of these excitons at the interface of CNT (5,0) and PbSe NW. Both carbon nanotubes (CNT) and semiconducting nanowires (NW) have been extensively researched; however, relatively little research has been conducted on these two systems in conjunction (**Figure 1**). It is known that CNTs and NWs both absorb light, conduct electricity in axial directions, and generate charge transfer states the interface, which could lead to potential breakthroughs in flexible electronic, optoelectronic and photovoltaic devices.

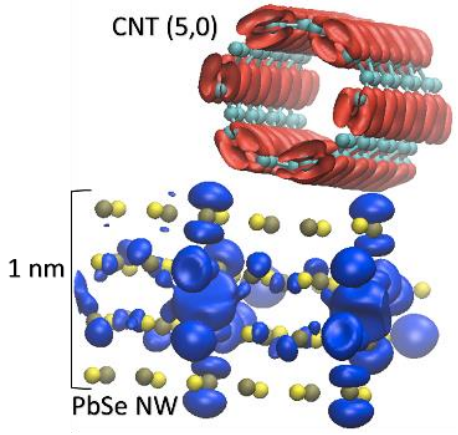

Figure 1: Atomic model of interface and molecular orbitals HO_{CNT} (red), LU_{PbSe} (Blue)

We used unrestricted density functional theory (DFT), and Perdue Burke Ernzerhof (PBE) in Vienna Ab-initio Simulation Package (VASP) software as a way to characterize the optical absorption spectra, modeled in the basis of Kohn-Sham orbital pairs, occupied and unoccupied. Superpositions of such pairs, both localized on CNT, are responsible for lowest and most intense optical transitions. Superpositions of pairs both localized on NW are contributing to the lowest and most intense optical transitions. Superpositions of "hybrid pairs" are responsible for dark charge transfer states in the non-radiative dynamics. Spatially localized states serve as initial states, while the hybrid states can be occupied as a result of non-radiative relaxation processes. This material is based upon work supported by the National Science Foundation under CHE - 1413614 "Theoretical Insights into Chemical Functionalization of Carbon Nanotubes: from Chirality Separation to Photoexcited Dynamics "