"Stretching the Limits of Carbon Through PbSe Quantum Dot Sensitization of Nanotubes"

Jeffery D. Mottishaw, Dmitri S. Kilin, and Haoran Sun

Department of Chemistry, University of South Dakota, Vermillion, SD 57069

PbSe-based quantum dots have been shown to be excellent sensitizers in a variety of optoelectronic device configurations, such as dye-sensitized solar cells, bioimaging, and targeted drug delivery[1]. However, for solar applications, optimizing the interaction between these dots and inexpensive acceptor materials, is crucial for their widespread application. Carbon nanotubes, a 1D allotrope of graphene, has excellent acceptor properties and well-established synthetic procedures. In order for optimal solar device performance, one needs to maximize the donor-acceptor interface charge transfer rates, and minimizing the loss of exciton pairs to non-radiative decay pathways[2]. Several representative configurations of PbSe quantum dots adsorbed to semiconducting carbon nanotubes through both covalent and non-covalent linkers will be investigated using DFT-based methods in the Vienna Ab Initio Simulation Package to determine optical properties, charge transfer rates, and losses due to dissipation through an ab inito molecular dynamics approach[3]. It is expected that this research will guide experimentalists in the development of high-performance optoelectronic devices.

[1]Douglas P. Shepherd, Justin B. Sambur, Yong-Qi Liang, Bruce A. Parkinson, and Alan Van Orden, *Journal of Physical Chemistry C* **116** (39), 21069 (2012).

[2]Iek-Heng Chu, Dmitri S. Kilin, and Hai-Ping Cheng, *Journal of Physical Chemistry C* **117** (35), 17909 (2013).

[3]Jeffery D. Mottishaw, Dmitri Kilin, Hai-Ping Cheng, Valentin V. Karasiev, Qi Hua Fan, and Haoran Sun, *Molecular Physics*, Ahead of Print (2013).