DFT study on the charge transfer excited states of organic molecules

Tunna Baruah[1,2]
[1]Department of Physics
[2]Computational Science Program
University of Texas at El Paso
El Paso, TX, 79968

The charge transfer excitation plays a crucial role in photovoltaics and photocatalysis processes. The description of charge transfer excited states with vanishingly small transition dipole has been in focus in recent years. We use a delta-SCF type method within density functional theory to predict the charge transfer excitation energies of organic donor-acceptor molecules. The method was first tested on a set of small molecular conjugates of electron donor and acceptor molecules. Our calculated values of the charge transfer excited states show a mean absolute deviation of 0.09 eV from experiment [1]. Applications of the method to several other large systems which are used as active material for organic photovoltaics such as porphyrin-fullerene dyads [2,3], carotene-porphyrin-fullerene triad [4], heptad, dye-attached fullerenes with P3MT polymers show promising results and will be presented. The agreement between our calculated values and experiment for these materials show the potential of the method for predictive screening of materials for photovoltaic properties.

References:

[1]T. Baruah, R. R. Zope, M. Olguin, J. Chem. Phys. 137, 084316 (2012).
[2] R. R. Zope, M. Olguin, T. Baruah, J. Chem. Phys. 137, 084317 (2012).
[3] M. Olguin, R. R. Zope, T. Baruah, J. Chem. Phys. 138, 074306 (2013).
[4] T. Baruah, M. Pederson, J. Chem. Theo. Comp, 5, 834 (2009).
[5] L. Basurto, R. R. Zope, T. Baruah, (http://arxiv.org/abs/1306.2627).