DFT study on the excited states of organic donor-acceptor molecules

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The open circuit voltage of an organic photovoltaic is depends on the charge-transfer excitation energies of the active material which consists of an electron donor and acceptor moieties. We use a perturbative delta-SCF method within density functional theory to predict the charge transfer energies of organic molecular conjugates. The method was 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] and also to a large heptad molecule [5] will be presented and discussed. The agreement between our calculated values and experiment for these applications show the potential of the method for predictive screening of materials for photovoltaic properties.

References:

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