
The ability of donor-acceptor (D-A) type polymers to control the positions of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals makes them a popular choice for organic solar cell applications. The alternating D-A pattern in a monomer leads to a weak electronic coupling between the constituent monomers within the polymer chain. Exploiting the weak electronic coupling characteristics, we developed a method to efficiently calculate (1) the electronic properties and (2) the optical gap of such polymer chains. The electronic properties (HOMO and LUMO energies, ionization potential, electron affinity, and quasiparticle gap of an oligomer of any length up to an infinitely long polymer) of the D-A polymers are predicted by combining density functional theory calculation results and a tight-binding model. The weak electronic coupling implies that the optical gap of the polymer is size-independent, and thus, it can be calculated using a monomer. We validated the methods using a set of 104 polymers by checking the consistency where the electronic gap of a polymer is larger than the optical gap. Furthermore, we establish relationships between the results obtained from more accurate, yet slower methods (i.e., B3LYP functional, singlet-ΔSCF) with those obtained from the faster counterparts (i.e., BLYP functional, triplet-ΔSCF). Leveraging the found relationships, we propose a way in which the electronic and optical properties of the polymers can be calculated efficiently while retaining high accuracy. The use of the tight-binding model combined with the approach to estimate more accurate results based on less expensive simulations is crucial in the applications where a large volume of computations needs to be carried out efficiently with sufficiently high accuracy, such as high-throughput computational screening or training a machine-learning model.

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