Development of the Fragment-Based GW+Bethe-Salpeter Equation Method for Applications to Organic Materials

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Organic electronics based on π-conjugated molecules or polymers have attracted considerable attention due to their attractive features. Predicting the charged-transport levels or optical excitations is essential for understanding the electronic processes governing the device operation and for rationally designing novel materials. The successful theoretical descriptions of charged and neutral excited states requires an accurate quantum mechanical method: in addition, the effects of polarizable environment must be properly taken into account. Here, we present a large-scale GW implementation based on the fragment molecular orbital method [1,2]. The implementation is based on the fragmentation approximation of the polarization function [3] and the combined GW and Coulomb-hole plus screened exchange approximations for self-energies [4]. Our fragment-based method can describe the state-specific polarization effect and the delocalization of charge and excited states on the same footing. The fragment-based GW is demonstrated by applications to an organic semiconductor thin film and a donor/acceptor interface structure. We highlight the impact of the induced polarization effects on the charged and neutral excitations in the organic semiconductors.

References

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