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Charge-Transfer Excitation within a Hybrid-(G)KS Framework through Cartesian Grid DFT

Raj Roy, Abhisek Ghosal, and Amlan K. Roy*

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Abstract

Organic molecules that exhibit charge-transfer (CT) excited states are known to play an important role in processes linked to electron transfer properties and molecular conductance. In this article, we present a simple technique based on "Becke's excitation theorem" that offers an accurate picture of these electronic states. It expresses the correlated energy splitting between triplet and its corresponding singlet states by a two-electron integral, which is numerically evaluated by our recently developed strategy on Cartesian grid. We first examine the consistency of our adopted numerical strategy to evaluate the integral with the original prescribed technique. Then we assess the method on weakly bound CT complexes with three different functionals (BLYP, B3LYP, and LC-BLYP). The accuracy on asymptotic limit of CT excitation is also explored. Finally in order to illustrate the strength and feasibility, it is further extended to a few "challenging" molecules. The method, when employed with hybrid B3LYP functional, turns out to be quite accurate to describe CT excitation energy.