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Charge-transfer excited states using a constrained density functional method[1] MARCO OLGUIN, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — Growing interest in characterizing charge-transfer (CT) processes inherent in many chemical interactions, such as metal surface-adsorbate catalysis or light harvesting processes, has prompted a demand for practical electronic structure methods with sufficient accuracy to describe the excited-states of large systems. The widely used time-dependent density functional formalism shows limitations in describing CT excited-states. In this study, we employ a recently developed constrained excited-state method to estimate the energies of singly excited particle-hole states. The applied constraint in this approach is the orthogonality between the ground and excited-states. The expense involved in the calculation of each excited state is comparable or slightly less than that for the ground state. A comparison of the gas-phase CT excitation energies for a set of aromatic donor with TCNE acceptor show excellent agreement with experimental values. Its application to the CT excited states for a light harvesting C60-porphyrin-beta-carotene triad demonstrates the applicability of this approach to large systems. The performance appraisal of this method for a large number of excited states including core excitation will be presented and further improvements will be discussed.

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