Energy decomposition analysis method for intermolecular interactions with excited states

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Understanding the nature of intermolecular interactions with excited states is highly expected but challenging. As quantitive analysis tools for intermolecular interactions, most of energy decomposition analysis (EDA) methods are restricted to the interactions in the ground states. In this talk, an EDA method for intermolecular interactions with excited states, called GKS-EDA(TD), is proposed based on time-dependent generalized Kohn-Sham theory (TD-GKS) theory. As an extension of GKS-EDA, GKS-EDA(TD) divides the total interaction energy in excited states into electrostatic, exchange-repulsion, polarization and correlation/dispersion. The nature of intermolecular interactions, including hydrogen bond, OH$\cdots\pi$, and $\pi\cdots\pi$, in their low singly excited states, are investigated. These test examples show that GKS-EDA(TD) is capable of analyzing various intermolecular interactions with different excitation modes, including local excitation, charge transfer excitation and mixed excitation mode.

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