How to understand intermolecular interactions and chemical bonds in complex systems

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Intermolecular interactions and chemical bonds in complex systems, which are related to variable spin states, excited states, and environment effects, are important but challenging. In this talk, first, I will present a brief review of our energy decomposition analysis (EDA) methods for complex systems, which were developed based on KS-DFT (GKS-EDA),[1,2,3] tight-binding DFT (DFTB-EDA),[4] and valence bond theory (VB-EDA). [5] Secondly, I will introduce a density matrix strategy-based EDA method, called DM-EDA, [6] for n-body intermolecular interactions. Different from traditional EDA methods, instead of intermediate state wave function, the EDA terms in DM-EDA are expressed in the forms of density matrix. New insights would be provided when the results of different density matrices are compared. Finally, the standalone EDA software developed in our group, called XEDA, will be introduced.

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