A valence bond based energy decomposition analysis scheme and its application to charge shift bonds

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Abstract

A new energy decomposition analysis (EDA) scheme based on valence bond (VB) wave function, called VB-EDA, is presented.[1] By this scheme, the total interaction energy by valence bond calculations.is decomposed into frozen, charge transfer, polarization and dynamic correlation terms. The advantages of VB-EDA over the currently existing MO- or DFT-based EDA schemes are as following: First, polarization and charge transfer in VB-EDA are well separated; second, the analysis results are not sensitive to basis sets, which means that a relatively small basis set is adequate. This scheme can be used for various intermolecular interactions, ranging from weak non-covalent interactions to strong covalent bonds. Using VB-EDA, a series of charge shift (CS) bonds is studied and discussed.

Reference and notes

[1] Zhang, Y., Chen, S., Su, P., Wu, W. J. Phys. Chem A. In submission.