Path dependency of Energy Decomposition Analysis: Collective bonding as a corner case

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Energy Decomposition Analysis (EDA) is a technique of computational chemistry for classification of chemical bonds or interactions.
It partitionates bonding energy into meaningful components: preparation energy, electrostatic interaction, Pauli repulsion and orbital interaction energy. The calculation consists of squashing wavefunctions of relaxed fragments to the geometry of the molecule, followed by antisymmetrization and relaxation. It has been demonstrated earlier that the components depend on the choice of "reaction" path[1,2].
Alternative to EDA might be Quantum Theory of Atoms in Molecules (QTAIM) with Interacting Quantum Atoms (IQA) method of partitioning of total energy and different definition of interactions. According to this definition, the components are guaranteed to be just a function of state since the calculation doesn't depend on any construction.
Published results of my other project[3] have been challenged by a competing team using arguments involving EDA calculation in situations where it hit its limitations.
Our project on proper explanation of the limitations of EDA method

References

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