Stepwise Energy Decomposition Analysis: Calculation with simple molecules using modified GAMESS code

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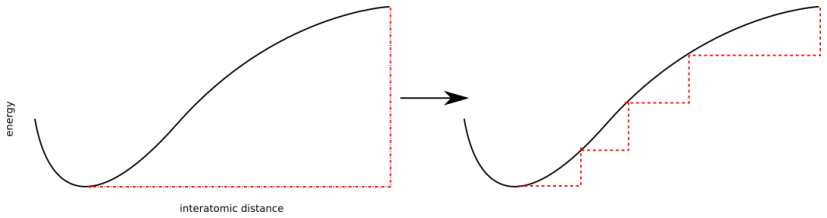

Bonding energy characterizes chemical bonds and other interatomic interactions. Compuational chemistry provides several methods of interaction characterization. Energy Decomposition Analysis (EDA) partionates bonding energy into components: preparation energy, electrostatic interaction, Pauli repulsion and orbital interaction energy. The caclulation consists of squashing wavefunctions of relaxed fragments to the geometry of the molecule, followed by antisymetrization and relaxaton.
Sola and Poater demonstrated different results for different orders of composition for multi-component structures.
Our aim is to demonstrate the limitations of the EDA method on supersimple diatomic molecules. The plan was to split the calculation into several steps instead of just one. We preyed on the source code availability of computational software GAMESS. The tweaked code can perform the stepwise EDA. Results with H2, Li2. LiF, LiCl, N2 are shown.

References

1. Solà, M., Duran, M., Poater, J. “The energy components of the extended transition state energy decomposition analysis are path functions: the case of water tetramer.” Theor Chem Acc 140, 33 (2021). doi:10.1007/s00214-021-02730-3
2. Poater, J., Andrada, D. M., Solà, M. & Foroutan-Nejad, C. Path-dependency of energy decomposition analysis & the elusive nature of bonding. Phys. Chem. Chem. Phys. 24, 2344–2348 (2022) doi:10.1039/D1CP04135E