On the Applicability of Various Partitioning Schemes to Intermolecular Interactions

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An availability of partitioning schemes for molecular energies and properties increases considerably the explanatory and predictive power of computational chemistry. Such schemes, although often not strict, are nevertheless physically convincing and allow in many cases to answer important practical questions, concerning e.g. the substituent dependence of stability and reactivity. Some of these partitioning schemes were designed especially for intermolecular interactions, like F-SAPT approach [1], while for other methods the intermolecular interactions are treated on the same footing as e.g. covalent ones (quantum theory of atoms-in-molecules – QTAIM [2], interacting-quantum atoms – IQA [3], etc.). Yet another philosophy stays below the Molecular Fragmentation (MF) models (see e.g. the Systematic MF from [4]), which can also be applied to calculate and to partition intermolecular interaction energy. Here we present a study of suitability of these methods to explain the nature of intermolecular interactions and its dependence on a detailed molecular structure for several nontrivial test cases, like complexes with boron/nitrogen doped analogs of benzene [5] or complexes with calixarenes [6].

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