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Intrinsic Bond Energies: A real space point of view

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A not completely extinguished fire on the nature of the chemical bond in the C₂ molecule [1] has re-opened several dormant fronts on the interpretation of bond energies. One of these regards whether we should measure bond strengths with respect to the ground states of the isolated fragments that become bonded, leading to standard bond dissociation energies (BDE), or if appropriately “prepared for bonding”, i.e. excited, states should be used instead. The latter view provides larger bond energies, which are usually called intrinsic bond energies (IBE) [2]. Here we examine this problem from a real space partitioning point of view, using the Interacting Quantum Atoms (IQA) approach [3] and electron number distribution functions (EDF) [4]. In IQA, the molecular energy is exactly written as a sum of atomic or fragment self-energies and interatomic (or inter-fragment) interaction energies. The evolution of self-energies along bonding coordinates allows for the identification of the proper atomic/fragment state that reflects the actual electronic state of each fragment in-the-molecule, which can then be used to properly define IBEs. Some results on methane, ethene, ethyne, dinitrogen, and dicarbon will be shown.

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