Some applications and developments within the QTAIM and IQA topological methods

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The Quantum Theory of Atoms in Molecules (QTAIM)[1] and the electronic energy partition in accordance with the Interacting Quantum Atoms (IQA)[2,3] approach are important methods within the realm of quantum chemical topology. Both QTAIM and IQA have provided valuable insights about many different important systems and phenomena in chemistry. In that regard, this seminar addresses the utilization of IQA to the analysis of cooperative[4] and anticooperative[5] effects of hydrogen bonding together with the combined use of linear response TDDFT and QTAIM to the analysis of molecules in electronically excited states[6]. The foundations of this last application i.e., the computation of TDDFT relaxed electron densities obtained after solving a Z-vector equation are considered as well. Finally, the inclusion of dynamic electron correlation in the IQA electronic energy partition through the use of Hartree-Fock/Coupled Cluster (CC) transition density matrices[7] and a subsequent improvement by the use of the CC Lagrangian[8] are discussed. It is to be hoped that the developments presented in this talk will increase the applicability of IQA and QTAIM and thereby providing important tools in the field of quantum chemical topology.

References

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