# Quantum Interference Provides a Unified Description of Chemical Bonding

Felipe Fantuzzi, Thiago Messias Cardozo, Marco Antonio Chaer Nascimento

Instituto de Química, Universidade Federal do Rio de Janeiro, Brazil.
chaer01@gmail.com

Although the chemical bond is usually considered to be a very well established concept, its origin and nature are still subject to much discussion [1-4]. It is well known that the minimum in the potential energy surface (PES) responsible for the bond in a stable system is followed by a decrease of potential energy, and a rise of kinetic energy, as required by the virial theorem. However, this analysis does not provide a model for explaining bond formation. Since total kinetic and potential energies are a direct consequence of the form of the total electronic density, the question of why the electronic density of a bonded molecule changes in such a way that results in an energy drop is unanswered by these quantities[1-4]. This can be understood through an alternative energy partitioning, derived from a density partitioning in quasi-classical and interference contributions [5-9], by recognizing that the quantum mechanical interference effect changes the electron density in a way as to reduce the energy and promote the formation of chemical bonds. The results obtained for a variety of diatomic and polyatomic molecules based on this energy partitioning attest that quantum interference plays a definite role in the formation of chemical bonds, irrespective of being classified as covalent, polar or even "ionic" [5-9]. Moreover, the developed approach provides a unique way of obtaining the total interference energy of a molecule in terms of bond contributions. Besides that, it can be shown that bond interference energies have characteristic values for a given pair of atoms in similar chemical environments [9]. In conclusion, the analysis of the chemical bond from the quantum interference perspective provides a unified description of chemical bonding (CNPq, FAPERJ).
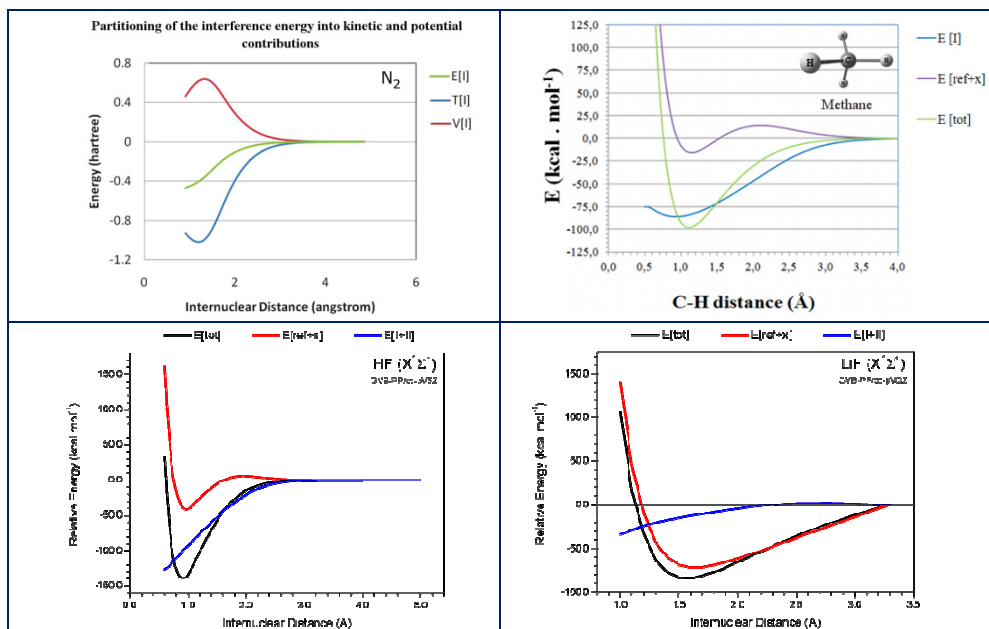
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