

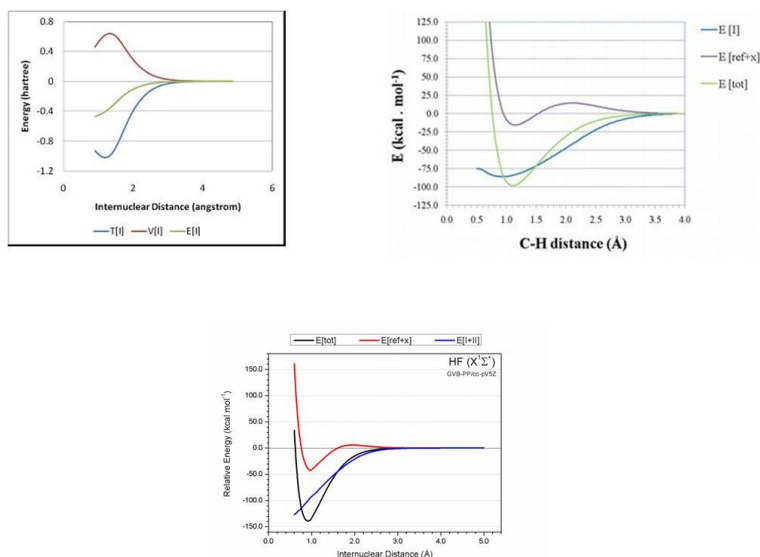
Quantum Interference Provides a Unified Description of Chemical Bonding

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Although the chemical bond is usually considered to be a very well established concept, its origin and nature are still subject to much discussion¹⁻⁴. 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 quantities¹⁻⁴. This can be understood through an alternative energy partitioning, derived from a density partitioning in quasi-classical and interference contributions⁵⁻⁹, 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 chemical bonds, irrespective of being classified as covalent, polar or even “ionic”, are formed only in the presence of quantum interference⁵⁻⁹. 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 environments⁹. In conclusion, the analysis of the chemical bond from the quantum interference perspective provides a unified description of chemical bonding (CNPq, FAPERJ).



- [1] Ruedenberg, K. *Rev. Mod. Phys.* **1962**, 34, 326–376.
- [2] Wilson, C. W.; Goddard, W. A. *Chem. Phys. Lett.* **1970**, 5, 45–49.
- [3] Kutzelnigg, W. *Theoretical Models of Chemical Binding*; Maksic, Z. B.; Springer: Heidelberg, Germany, 1990; Vol. 2, p 1.
- [4] Nascimento, M. A. C. *J. Braz. Chem. Soc.* **2008**, 19, 245–256
- [5] Cardozo, T. M.; Nascimento, M. A. C. *J. Chem. Phys.* **2009**, 130, 104102–8.
- [6] Cardozo, T. M.; Nascimento, M. A. C. *J. Phys. Chem. A* **2009**, 113, 12541–8.
- [7] Cardozo, T. M.; Nascimento Freitas, G.; Nascimento, M. A. C. *J. Phys. Chem. A* **2010**, 114, 8798–8805.
- [8] Fantuzzi, F.; Cardozo, T. M.; Nascimento, M. A. C. *Phys. Chem. Chem. Phys.* **2012**, 14, 5479–5488.
- [9] Vieira, F.S., Fantuzzi, F.; Cardozo, T. M.; Nascimento, M. A. C. *J. Phys. Chem. A* (DOI: 10.1021/jp4005746)