

Understanding Chemical Bonding and Aromaticity From Electronic Delocalization Descriptors

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Interactions between electrons determine the structure and properties of matter from molecules to solids. Therefore, the understanding of the electronic structure of molecules will enable us to extract relevant chemical information. Since the work of Lewis,¹ the concept of electron pair has been placed at the epicenter of the discussion about the properties of chemical bonding. Hence, the pair density, that accounts for the correlated motion of a couple of electrons, has been very important in the interpretation of electronic structure. The pair density and its related quantities, such as the concept of Fermi Hole or the exchange-correlation density have been widely used to elucidate the nature of chemical bonding in a plethora of systems.

In chemistry, global molecular properties are as important as the properties of a given atom or region of the molecular space. The partition of molecular space into different regions helps us to unravel how the electrons are localized in a specific region or which is the number of electrons shared among two or more regions of the space. In this talk we focus our attention on the analysis of chemical bonding and aromaticity by means of the electron sharing indices (ESI)² based on the Quantum Theory of Atoms-in-Molecules (QTAIM)³. In particular, we will see how the ESI account for the effects of conjugation and hyperconjugation in some simple organic compounds, and how they can be used to describe the aromaticity of the low-lying singlet and triplet excited states in some archetypical aromatic and antiaromatic compounds.

[1] Lewis, G. J. *Am. Chem. Soc.* 1916, 38, 762

[2] Poater, J.; Duran, M.; Solà, M.; Silvi, B. *Chem. Rev.* 2005, 105, 3911.

[3] Bader, R.W.F. *Atoms in Molecules - A Quantum Theory*, International Series of Monographs on Chemistry, No. 22. 1990.