Topological analysis of some electron density derived Functions

William Tiznado

Departamento de Ciencias Químicas, Facultad de Ecología y Recursos Naturales, Universidad Andrés Bello, Av. República 275, Santiago-Chile.

The Atoms in molecules (AIM) analysis proposed by Bader is a powerful tool in describe and rationalize some important concepts of the chemistry like chemical bond, electron density polarization in molecules, among others. Inspired in this theory most recently the topological analysis of other functions obtained by quantum calculations were proposed, some of they are very used by its simple interpretation as the Electron Localization Function (ELF).

In this talk we will present the topological analysis of three functions, the Fukui function, the ELF_{σ} and ELF_{π}. The first function is related to local reactivity of the systems, this form of evaluate the Fukui allows us obtain attractors which identify regions (basin) with chemical reactivity interpretation, core, bonding or valence basins. The second and third functions are the sigma and pi electronic contributions to the ELF. The bifurcation analysis of these functions is good aromaticity descriptor, and has been successfully applied to describe and assign aromaticity of organic and inorganic systems