

Microsymposium

MS19.O03

Insights on spin-polarization via the spin density Source Function

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The Source Function (SF) [1-3], enables one to view chemical bonding and other chemical paradigms from a new perspective and using only information from the electron density observable and its derivatives. We show how this tool may be straightforwardly applied to another important observable, the electron spin density, which analogously to the electron density may be locally interpreted in terms of a cause-effect relationship of contributions from the atoms of a molecular or crystalline system. Application of the spin density SF to molecules in vacuo and to slab or crystals, is made possible through an extension (SPINSF code) of our electron density SF code for molecules and through a progress-version of the TOPOND code, respectively. The latter has now been fully integrated in the CRYSTAL-14 code, where it provides, via the keyword TOPO of the properties section of CRYSTAL-14, a complete charge density topological analysis according to the Quantum Theory of Atoms in Molecules. Analysis of the SF for the electron spin density implies the study of its Laplacian scalar field, which may be locally positive or negative even if the two composing densities, $\rho\alpha$ and $\rho\beta$, have both negative or positive Laplacian densities. When the latter bear the same sign, that of the spin density Laplacian depends on their relative magnitudes, that is on the relative concentration or dilution of $\rho\alpha$ and $\rho\beta$. Hence, in general, the local source for the spin density, LSs, greatly differs from the analogous function for the density, leading to large differences in their integrated atomic SF contributions. The combined study of LSs and of the spin density neatly reveals which are the molecular or crystal regions that are “ferromagnetically” or “antiferromagnetically” coupled and the local strength of such coupling. Applications to crystals of metal-complexes where the ligands play an innocent or a non-innocent role and to crystals of iron spin-crossover complexes are discussed.

[1] R.F.W. Bader, C. Gatti, *Chemical Physics Letters*, 1998, 287, 233-238, [2] C. Gatti, *Structure & Bonding*, 2012, 147, 193-286, [3] C. Gatti, *Physica Scripta* 2013, 87, 048102 (38pp)

Keywords: source function, spin density, magnetic coupling