A NOVEL VIEW ON ELECTRON LOCALIZATION

János G. Ángyán

CRM2, CNRS & Nancy University, B.P. 70239, F-54506 Vandoeuvre-lès-Nancy, FRANCE
email: angyan@crm2.uhp-nancy.fr

Point-wise characterization of electron localization/delocalization usually proceeds by functions, defined in terms of appropriately scaled dimensionless quantities. Tools like different variants of the electron localization function (ELF) have proven their tremendous usefulness to identify core, bonding and lone-pair regions in molecules or in solids and helped to understand even unconventional features of the electronic structure. Topological analysis of the ELF vector field leads to a partition to localization domains, over which a population analysis of the electron density can be subsequently performed. One may raise the question, whether it possible to construct a function, which not only reveals the presence of electron pair localization in a given region of space, like the ELF, but which, in the same time, is appropriate to perform a meaningful population analysis? Based on the recently established charge density reconstitution rule of the exchange-correlation hole [1] and by choosing an appropriate model hole centred on the barycentre of the physical hole, a new function has been constructed, which has the dimensions of a charge density, preserves the dipole moment and is able to display attractors around the centroids of the electron pairs. The new function, which can be named haystack function, since it collects the charge associated to electron pairs, like hay is raked in haystacks, can be regarded also as a fuzzy variant of the Wannier-center [2] representation of the electron pairs.


methane

benzene

carbon monoxyde