Development of new methods into the framework of Bader’s Theory and their application

Abstract:

The chemical behavior of atoms and molecules is entirely defined by the distribution of their electron density. It is by studying the electron density that key concepts of chemical importance come about, such as chemical bonding, reactivity, atomic hybridisation, and the existence of electric multipole moments. The last decades have seen the development of modern theories to study charge density and the most influential to date has been the quantum theory of atoms in molecules (QTAIM), developed by R.W. Bader and colleagues in the 1980s. At the heart of QTAIM there exists the central concept of atomic basins, which subdivide a molecule into regions that encase an atomic nucleus: an atom. With the success of Bader’s original theory a series of different topological tools were developed as source function (SF) (eq.1), delocalization indexes, Espinosa indexes, domain-averaged Fermi hole analysis and so on. A novel approach for SF was developed through its calculation from electron densities generated by plane wave (PW) methods. To show the validity of developed method on a series of test systems the results obtained at PW level were compared with those previously obtained through AE methods. Furthermore, a new topological tool is developed, the Bader energy density, $P_{BADER}$ (eq.2), which is introduced and applied to the study case of chemical reactivity $a$ priori of PH$_5$.

$$SF(r, \Omega) = -\frac{1}{4\pi} \int_{\Omega} d\mathbf{r}' \frac{\nabla^2 \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$  \hspace{1cm} (1)$$

$$P_{BADER}(\Omega) = \frac{E(\Omega)}{V(\Omega)}$$  \hspace{1cm} (2)$$

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