Physico-Chemical nanomaterials science

Modified patition ratio approach for searching and analyzing local orbitals in small carbon nanoclusters

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For nanoclusters and solids, the localization analysis of one-electron states, or molecular orbitals (MOs), can be performed by using the so-called partition ratio (PR) index. To this PR approach, we add for each MO the new index which we define as an average fluctuation of the inverse PR (IPR) index. Typically, displays a significant sensitivity to any spatial irregularity in distributing MO over molecule.

We apply the thus extended analysis to various carbon nanoclusters treated here at the level of the semiempirical extended Hückel method. In this way, we study the localization of edge states in the graphene nanoflakes which we examined previously [1,2]. Other examples are related to nanodiamonds including negative nitrogen-vacancy (NV^-) color centers as well. Specifically, we consider the pristine diamondoid $C_{190}H_{110}$ and corresponding NV-color center $C_{188}H_{110}N^-$. We show that in the pristine diamondoid the highest occupied MO (HOMO) is a rather delocalized bulk orbital with a moderate amount of the index. Simultaneously, in the color center we see a strong localization of HOMO near the cluster vacancy. In this case, a sharp peak in the plot is observed, thus reflecting clearly a large orbital irregularity in HOMO.

The above examples and many others given in the present report allow us to assert that the proposed scheme is quite practical for huge clusters, permitting one to rapidly detect the orbitals with unusual non-uniform distribution.

1. *Luzanov A. V.* Measures of unpaired electrons for large conjugated systems // J. Struct. Chem.-2014.-**55**, N 5.-P. 799-808.
2. *Luzanov A. V.* Effectively unpaired electrons in bipartite lattices within the generalized tight-binding approximation: application to graphene nanoflakes // Funct. Mater.-2014.-**21**, N 4.-P. 437-447.