Domain Averaged Fermi hole Orbitals for Extended Systems

Baranov, A.I.
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DOMAIN-AVERAGED FERMI HOLE ORBITALS FOR EXTENDED SYSTEMS

Alexey I. Baranov, Miroslav Kohout, Robert Ponec

Max Planck Institute for Chemical Physics of Solids, Noethnitzer Strasse, 40, 01187, Dresden, Germany
Institute of Chemical Process Fundamentals, Czech Academy of Sciences, Prague 6, Suchdol 2, 165 02, Czech Republic
*E-mail:*baranov@cpfs.mpg.de

The analysis of the domain-averaged Fermi holes (DAFH) in terms of the orbital-like functions [1] was successfully applied to many simple as well as complex molecular systems at different levels of theory to gain visual and chemically appealing representations of bonding situations, making it possible to establish a connection to orbital-like models and concepts in chemistry [2]. The realm of solids was however not subjected to this method of analysis up to know and even the accurate calculations of the delocalization indices for them were reported only recently [3]. Current contribution presents the results of DAFH orbital analysis for several simple model systems like hydrogen lattices as well as for prototypic real solids with covalent, ionic and metallic bonding.

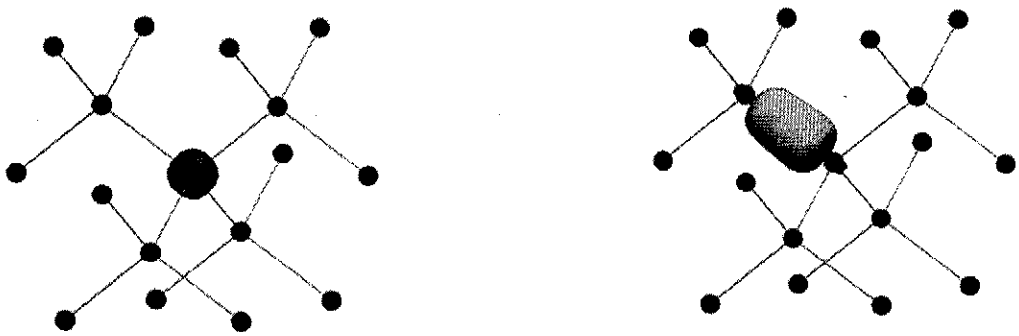

Fig. 1. DAFH orbitals for the diamond

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2. D. Tiana, E. Francisco, M. A. Blanco, P. Macchi, A. Sironi, Á. Martín Pendás Phys. Chem. Chem. Phys. 13, 11, 5068, 2011.

3. A. I. Baranov, M. Kohout J. Comp. Chem. 32, 10, 2064, 2011.