Nanoscale physics

Studies of sensing and storage capabilities of B(N)-doped carbon nanostructures by electronic structure calculations

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Carbon nano-structured materials are intensively studied as perspective materials for various applications, in particular gas sensing, and chemical passivation of toxic compounds. The capabilities of carbon materials in such applications can be efficiently predicted by the first-principles theoretical modeling of molecular adsorption of their surfaces.

Several cases of such prediction are demonstrated in this report. One of them is related to studies of potential applicability of undoped, B- and N-doped carbon nanotubes (CNTs) for elaboration of the working materials of gas sensors of hydrogen halide molecules HX (X = F, Cl, Br). Other are related with potential application of B(N)-doped carbon nano-structured materials for efficient removal and storage of toxic molecular oxyanions XO_4^{2-} (X = Cr, Mo, W). A DFT-based geometry-optimized calculations of the electronic structure of undoped, B- and N-doped CNTs of (3,3) and (5,5) chiralities, graphene sheets and other types of carbon nano-structures with adsorbed molecules are carried out within molecular cluster approach by Gaussian 03 program package [1]. Relaxed geometries, binding energies between the adsorbates and carbon nano-structures, charge states of the adsorbates and the electronic wavefunction contours were calculated and analyzed in the context of gas sensing and oxyanion storage applications. The optical absorption spectra of XO_4^{2-} anions adsorbed on the CNTs surfaces were also calculated and compared with corresponding experimental data.

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1 *M.J. Frisch, et al.* // Gaussian 03 (Gaussian, Inc., Wallingford, CT, 2003).

2 *Yu. Hizhnyi, S.G. Nedilko, V. Borysiuk, and V. A. Gubanov* // Int. J. of Quant. Chem. (2015) 115 1475-1482.