Nanostructured surfaces

Studies of N(B)-doped carbon nanotubes and graphene as promising materials for the removal of oxyanions

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The N(B)-doped carbon nanotubes (CNTs) and graphene are intensively studied at present as materials for efficient removal and storage of various toxic molecules. Efficient functionalization of CNTs can modify their physical and chemical properties, leading to the improvement of their performance for specific applications. Some studies have already indicated that functionalized CNTs are a promising for the removal of toxic heavy metals traces from water wastes. Mentioned task is an important environment related issue because oxyanions of heavy metals are toxic industrial pollutants and their removal from industrial wastes is a urgent problem [1]. Computational modeling of such molecular adsorption on the CNTs surfaces is a powerful tool what allows to predict some important properties of materials perspective for mentioned use.

Theoretical modeling of the XO_4^{2-} (X = Cr, Mo, W) molecular oxyanions adsorption on the surface both of undoped and B(N)-doped carbon nanotubes were analyzed as result of computational studies. A geometry-optimized calculations of the electronic structure of undoped, B- or N-doped CNTs of (3,3) and (5,5) chiralities with adsorbed XO_4^{2-} oxyanions of various hexavalent transition metals were carried out using Gaussian 03 program package [2]. Relaxed geometries, binding energies, charge states of the adsorbates and the electronic wave-function profiles were calculated and analyzed. Taken results are supplemented by calculations of the XO_4^{2-} oxyanions adsorption on B(N)-doped graphene sheets which are considered as model approximation for large-diameter CNTs.

An induction of the B(N) doping on the type of chemical bonding between XO_4^{2-} anions and CNTs is revealed. The results are discussed in relation with prospects of the adsorbent to remove toxic chromates from aqueous solutions.

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2. *Frisch M.J., Trucks G.W., Schlegel H.B., et al*. Gaussian 03 (Gaussian, Inc., Wallingford, CT, 2003).