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ADSORPTION CHARACTERISTICS OF Cr(VI) MOLECULAR ANIONS ON FUNCTIONALIZED CARBON NANOSTRUCTURES: A DFT INVESTIGATION

The Density Functional Theory (DFT)-based computations of the electronic structure of undoped, B- and N-doped CNT(3,3), CNT(5,5), six-walled CNT with (37,37) chirality of outer layer and graphene with adsorbed chromate anions were performed within molecular cluster approach. The CNT(5,5) with several surface groups including –COOH, –COO-, –OH and –NH3+ were also considered as adsorbents in order to study the influence of functionalisation on the adsorption properties of the CNT-based materials with respect to toxic anions of hexavalent chromium Cr(VI). Relaxed geometries, binding energies and charge differences of the adsorbed chromate anions were calculated using B3LYP correlation functional. Doping with B substantially decreased (by ~1.5 – 2.5 eV), while doping with N increased (by ~2 – 4 eV) the absolute values of binding energies relatively to corresponding adsorption cases on undoped CNTs in vacuo. The negative binding energies values were obtained for adsorption of CrO42- on functionalized CNTs in vacuo.

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