Removal of oxoanions of M^{VI} (M^{VI}=Cr, Mo, W) metals by carbon nanostructures: Insights into mechanisms from DFT calculations

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Streszczenie

Carbon nanostructured materials have been recognized as perspective adsorbents for removal of toxic anions of hexavalent metals M(VI) from surrounding media. The article reveals the peculiarities of such removal mechanisms at a single-molecule level. Adsorption of $M^{VI}O_4^{2-}$ (M^{VI} = Cr, Mo, W), $Cr_2O_7^{2-}$, and $HCrO_4^-$ anions on the surface of pristine, B(N)-doped, and functionalized by functional groups (_COOH, $_COO^-$, _OH, and $_NH_3^+$) carbon nanotubes (CNT) and graphene is studied in the density functional theory electronic structure calculations carried out in vacuo and *in aqua* using polarizable continuum model. It is found that neither pristine, nor B or N-doped CNTs can be efficient adsorbents of the anions in water. Functionalization of the CNT-based materials with oxygen- or ammonia-containing surface groups will allow creation of efficient adsorbents of Cr(VI) toxic anions at low pH levels of water solution. Whereas at high pH (> 6), only functionalization by ammonia-containing groups is feasible for this task.

Słowa kluczowe

adsorption, carbon nanostructure, hexavalent chromium, oxoanion

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