Computational and experimental studies of adsorption of $CrO_4$2-molecular anions on the surface of carbon nanostructures

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Streszczenie

Search for new adsorbent materials which can allow economically-efficient schemes of the heavy metal removal is a topical research task. The Density Functional Theory (DFT) computations of the electronic structures of undoped, B-and N-doped graphene sheets with adsorbed chromate anions CrO_4^{2-} were performed within molecular cluster approach. Relaxed geometries and binding energieswere calculated using B3LYP hybrid exchange-correlation functional. Oscillator strengths of electronic transitions of CrO_4^{2-} anions adsorbed on graphene surface were calculated by TD-DFT method. The optical absorption spectra of aqueous solutions containing mixes of carbon nanotubes and chromate anions were measured. The luminescence emission spectra of carbon nanostructures with adsorbed chromate anions deposited on silicon glass substrate were measured. Two stable configurations were found for adsorption of CrO_4^{2-} anions on undoped graphene sheets. The calculated energy of the lowest-energy transition of the adsorbed CrO_4^{2-} anion is reduced by 0.5 eV in comparison with corresponding transition energy of free anion. Spectra of optical absorbance and luminescence of the systems containing carbon nanostructures measured before and after adsorption of chromate anions reveal substantial difference that confirms the principal possibility of monitoring the CrO_4^{2-} anion adsorption on carbon nanostructures.

Słowa kluczowe

Adsorption, Carbon nanotube, Chromate anion, Electronic structure, Luminescence

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