

Computational studies of adsorption of toxic molecules and anions on the surface of doped and functionalized carbon nanotubes.

Autorzy

Viktor Borysiuk

Sergii G. Nedilko

Yuriy Hizhnyi

Andrii Shyichuk

Rok wydania

2019

Wydawca

Springer

Miejsce wydania

Cham

Strony

305-340

DOI

10.1007/978-3-030-17755-3_21

bookChapter.title

Nanophotonics, nanooptics, nanobiotechnology, and their applications : selected proceedings of the 6th International Conference Nanotechnology and Nanomaterials (NANO2018), August 27-30,2018, Kyiv, Ukraine.

ISBN

Streszczenie

Carbon nanotubes are perspective adsorbents for removal of toxic pollutants from surrounding media. The electronic structure-related computational modeling of adsorption has been recognized as a powerful tool for prediction of adsorption capabilities of real CNT-based materials. This chapter describes application of such computational modeling to two perspective applications of the CNT-based materials: (a) elaboration of the resistivity sensors of hydrogen halide molecules HX (X = F, Cl, Br) which are toxic industrial gaseous pollutants and (b) removal of toxic anions of M(VI) (M(VI) = Cr, Mo, W) metals from ambient atmosphere and water. Results of the density functional theory (DFT)-based electronic structure calculations of adsorption of HX molecules and M(VI)O₄²⁻, Cr₂O₇²⁻, and HCrO₄⁻ anions on the surface of pristine, B(N)-doped, and functionalized by functional groups (–COOH, –COO⁻, –OH, and –NH₃⁺) CNTs and graphene sheets are analyzed in the context of the mentioned applications. The influence of the tube structure and curvature, type of X, type of doping (B of N) on adsorption characteristics of “HX on CNT” system is analyzed and discussed in regards to elaboration of gas sensors. The influence of the CNT structure, B(N)-doping, and functionalization on absorption capabilities of CNTs with respect to anions of M(VI) metals is analyzed in terms of interatomic chemical bonds between the CNTs and adsorbed anions. This allowed making several important inferences regarding modification of the CNT-based materials for efficient removal of the anions from surrounding media. Possibility of detection of CrO₄²⁻ anions adsorbed the CNT surface by the spectroscopic technique is analyzed.

Słowa kluczowe

Carbon nanotubes, Electronic structure, Adsorption, Hydrogen halide, Molecular anions, Density functional theory

978-3-030-17754-6

Adres publiczny

Kolekcja

https://doi.org/10.1007/978-3-030-17755-3_21

Naukowa

Język

Angielski

Typ publikacji

Rozdział książki

Plik został wygenerowany dnia 2026-04-25 05:03:06

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/6JyZCCy>.