Inorganic Chemistry Communications xxx (xxxx) 110191

Contents lists available at ScienceDirect

Inorganic Chemistry Communications

journal homepage: www.elsevier.com/locate/inoche

Short communication

Detection of nitrotyrosine (Alzheimer's agent) by $B_{24}N_{24}$ nano cluster: A comparative DFT and QTAIM insight

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ARTICLE INFO

Keywords:
Nanocage
Fermi level
Work function
Electrical

ABSTRACT

A nano-sensor for nitrotyrosine (NT) molecule was found by studying the interactions of NT molecule with new $B_{24}N_{24}$ nanocages. It was calculated using density functionals in this case. The predicted adsorption mechanisms included physical and chemical adsorption with the adsorption energy of −2.76 to −4.60 and −11.28 to −15.65 kcal mol^{-1}, respectively. The findings show that an NT molecule greatly increases the electrical conductivity of a nanocage by creating electronic noise. Moreover, NT adsorption in the most stable complexes significantly affects the Fermi level and the work function. This means the $B_{24}N_{24}$ nanocage can detect NT as a Φ-type sensor. The recovery time was determined to be 0.3 s. The sensitivity of pure BN nanocages could be improved without additional expensive structural manipulations. After the NT had been absorbed into the nanocage, UV–Vis spectrum analysis revealed that the transmission wavelength shifted significantly toward 390.07 nm. Hence, a redshift occurs when the NT molecule gets near the $B_{24}N_{24}$ nanocage. According to the present study model, $B_{24}N_{24}$ nanocages are possibly promising devices for NT sensors based on their electronic and structural properties.

1. Introduction

To research low-dimension compounds in a solitary setting, carbon nanocage structures including fullerene, cages, nanocapsules, nanopolyhedra, nanotubes, cones, onions, and cubes are quite effective [1–4]. Additionally, it is anticipated that various electrical, magnetic, and optical properties such as Coulomb blockade, super magnetism, and photoluminescence will be represented by boron nitride (BN) nanostructured materials with a bandgap energy of 6 eV and non-magnetism [5]. Nanomaterials made of BN, such as BN nanotubes [6–18], BN nanocapsules [19], BN nanoparticles [20], and BN nanocages [21–25], have been studied extensively. These substances are thought to be advantageous mixtures for semiconductors with high heat resistance, insulator lubricants, and electronic tools. A few BN nanocages may also be useful in this application, according to theoretical predictions [26–29]. Boron is often employed as a component in combustible propellants and combinations due to the element's high volumetric calorific and gross value as well as the non-toxic combustion products it produces. Furthermore, the electrical properties of the boron nitride unit (BN) are identical to those of the bicarbon unit (CC), according to our understanding. It is thus an ideal material for nanotechnology applications because of its appealing properties. Boron nitride nanocages are now the subject of a significant amount of research, both empirically and numerically. BN fullerenes were successfully manufactured using a laser ablation technique for the very first time in the year 1998 [30]. Using the arc-melting method, Oku et al. [31] created

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https://doi.org/10.1016/j.inoche.2022.110191
Received 18 September 2022; Received in revised form 23 October 2022; Accepted 4 November 2022
1387-7003/© 20XX