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DFT computational study of trihalogenated aniline derivative's adsorption onto graphene/fullerene/fullerene-like nanocages, $X_{12}Y_{12}$ (X = Al, B, and Y = N, P)

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ABSTRACT

Adsorption of 2,4,6-tribromoaniline (BA), 2,4,6-trifluoroaniline (FA) and 2,4,6-trichloroaniline (CA) onto the surface of coronene/fullerene/fullerene-like nanocages was investigated by theoretical calculations. Due to the adsorption of BA/FA/CA, there are significant changes in chemical descriptors and nonlinear optical properties. Energy gap values of all nanoclusters are lowered, giving an increase in conductivity of complexes except for fullerene. All complex's ultraviolet visible wavenumber is blue-shifted and especially for fullerene complex, the values are very high. The enhancement of Raman intensities shows that it is possible to design a nanocage sensor for detecting these compounds by surface-enhanced Raman scattering (SERS).

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Introduction

There are major industrial and medical impacts of nanotechnology (Rad et al., 2019). In different uses, including cancer treatment, a large number of nanotechnology-based products such as nanopharmaceuticals are used (Farjadian et al., 2019). The most commonly known materials for the construction of nanoparticle carriers are polymers, liposomes, micelles and inorganic nanoparticles (Ali et al., 2011). Examples of nanoapplications for the beverages and food industry include encapsulation to allow improved ingredient stability and new tastes and textures to be created, engineered nanoparticles for regulated flavors and scent release, nanomodified surfaces that provide antibacterial properties and dirt repellence and nanostructured materials for air and water filtration materials (Cushen et al., 2012). Several developments in different fields of research have been made in recent years including small particles and nanostructured materials (Asadi-Ojaee et al., 2019; Dadashi Firouzjaei et al., 2020). To date, a large number of noble metal nanomaterials with various morphologies (balls, rods, flowers, sheets, cages, etc.) have been developed to meet the requirements of various research studies (Chimene et al., 2015; Mitragotri et al., 2015).

Nanocage refers to a three-dimensional nanomaterial with a hollow interior and a porous outer surface, which can conduct intramolecular assembly and external modification effectively (Pan et al., 2020). In designing and integrating portable and wearable sensors of the next generation, the cross-correlation between structural characteristics and functional properties of nanomaterials plays an important role as architectures of the single component devices are adequately developed (Prosa et al., 2020). The use of reconstituted high-density lipoprotein nanoparticles for the delivery of therapeutic compounds for cancer treatment has been comprehensively studied (Chaudhary et al., 2019; Lacko et al., 2015; Raut et al., 2018). Nanotubes, nanocones and nanoclusters are all made up of these different kinds of nanostructures as potential candidates to build a new generation of sensors and drug carriers (Jafari et al., 2021; Khodashenas et al., 2020). Studies show that reconstituted high-density lipoprotein serves as a means of drug delivery of compounds into macrophages and atherosclerosis plaques (Zhang et al., 2017). A nanorobot for the controlled delivery of the widely used drug thrombin to cause tumor infarction and necrosis locally in tumor vessels was reported by Li et al. (2018, 2020).

In analytical chemistry, electrochemical analysis, biological sensing and detection, a number of surface-enhanced Raman scattering (SERS) semiconductor technology applications have been recently reported (Wang & Guo, 2020). Theoretical adenine adsorption on borophene nanosheet was studied by Sabokdast et al. (2020). Owing to electron exchange in the molecules-nanomaterial systems, the electrical conductance of the resulting complex and other electronic properties are subject to change that can be defined as a possible sensor (Padash et al., 2019, 2018). Because of their physical and chemical properties, nanocages very attractive type of structure specifically the smallest HOMO-LUMO gap (Naderi et al., 2017; Sherafati et al., 2018). Analysis of literature shows that

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