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ORIGINAL PAPER

A computational study on the potential application of $Ca_{12}O_{12}$ cluster for sensing of fungicide molecule

Mustafa M. Kadhim[1] · Taleeb Zedan Taban[2] · Rasha Fadhel Obaid[3] · Haider Abdulkareem Almashhadani[4,5] · Mohanad Hatem Shadhar[6] · Ghadeer Sabah Bustani[7] · Ahmed Mahdi Rheima[8] · Ali Mohamadi[9]

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Abstract

Density functional theory calculations are employed to investigate the impact of edifenphos molecule on the reactivity and electronic sensitivity of pure calcium oxide (CaO) nanocluster. The strong adsorption of edifenphos molecule on CaO nanocluster occurs by the sulfur head of the adsorbate, and the amount of the energy of this adsorption is around − 84.40 kcal/mol. The adsorption of edifenphos molecules results in a decrease in the values of E_g of CaO from 4.67 to 3.56 eV, as well as an increase in the electrical conductance. Moreover, the work function of CaO nanocluster is significantly affected, which changes the current of the field emission electron. Eventually, the recovery time is calculated around 99 ms at ambient temperature for the desorption process of edifenphos from CaO nanocluster surface. Based on the obtained results, CaO nanocluster could be considered a suitable sensor for edifenphos molecule.

Keywords Edifenphos · Charge transfer · Recovery time · CaO nanocluster · Sensor

Introduction

In 1985, fullerene (C60) was discovered by the efforts of Kroto et al. (1985). Following this discovery, widespread investigations have been dedicated to the development of novel materials with high stability that are almost/or spherical in shape and are called nanoclusters or nanocages. Between all nanocage structures, the $(XY)_n$ (n = 12) structure has attracted the attention of research groups, which is the most stable one (Xu et al. 2006; Wu et al. 2021; Yang et al. 2021). Although this structure follows the law of tetragonal, there is no plausible explanation for this exceptional configuration. $(XY)_{12}$ nanocluster resemble a shortened octahedron that includes six squares and eight hexagons. One of the most well-known $(XY)_{12}$ clusters is $B_{12}N_{12}$. The $B_{12}N_{12}$ has been identified through high-resolution transmission electron microscopy (HRTEM) images (Golberg et al. 1998). However, it was studied via mass spectrum previously (Oku et al. 2004). Based on theoretical investigations, $B_{12}N_{12}$ nanocage has been considered to assess its advantages as a sensor for the detection of nitric oxide (Beheshtian et al. 2012a; Li et al. 2022a; Chen et al. 2022; Obireddy and Lai 2021), NO_2 (Beheshtian et al. 2012b), and CO_2 (Beheshtian et al. 2011), As (III) and As (V) removal (Beheshtian et al. 2013; Li et al. 2022b, c; Jia et al. 2022), and H-storage (Giri

✉ Ali Mohamadi
alimodi326@gmail.com

Mustafa M. Kadhim
Mustafa_kut88@yahoo.com

1 Medical Laboratory Techniques Department, Al-Farahidi University, Baghdad, Iraq

2 Laser and Optoelectronics Engineering Department, Kut University College, Kut, Wasit 52001, Iraq

3 Department of Biomedical Engineering, Al-Mustaqbal University College, Babylon, Iraq

4 Dentistry Department, Al-Rasheed University College, Baghdad, Iraq

5 Medical Laboratory Techniques Department, Al-Turath University College, Baghdad, Iraq

6 Department of Civil Engineering, Dijlah University College, Al-Masafi Street, Baghdad 00964, Iraq

7 College of Dentistry, The Islamic University, Najaf, Iraq

8 Department of Chemistry, College of Science, Mustansiriyah University, Baghdad, Iraq

9 College of Science, Islamic Azad University, Mashhad, Iran

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