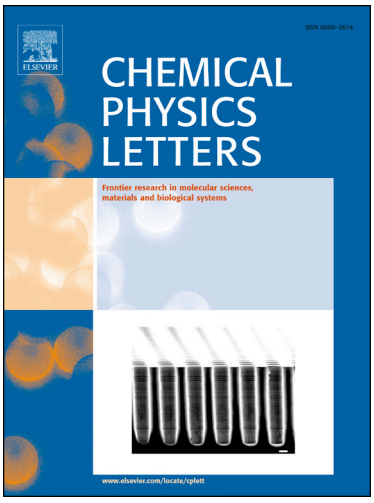

Research paper

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Adsorption, Intercalation and Sensing of Helium on Yttrium Functionalized Open Edge Boron Nitride: A First principle DFT and TDDFT Study

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Abstract

Open edge BN boron-nitride has a stable graphene-like structure, which could be doped by a range of impurities, so the band gap could be tuned. The optical, electrical, physicochemical properties, NBO and electron density of open edge BN that is doped by Yttrium was evaluated using DFT method as a sensor for He gas. Here, was applied HSE1PBE method exchange correlation and LANL2DZ. The density of states and natural bond orbital analysis calculated have depicted that the band gap of BN-Y flake after sensing He gas and it has shown change from 1.66→2.42eV. The UV-Vis absorption in λ_{max} area showed a significant red-shift that it is an appropriate parameter to recognize He molecule.

Keywords: Boron Nitride; BN-Y flake; Helium adsorption; NBO analysis; Physicochemical properties; Molecular modeling.

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1. Introduction

The development of chemical sensors is a field, which it requires great collaboration between the pure and applied sciences (1). A sensor detects events or changes in some calculable quantities and provides a corresponding output, typically as electrical or optical signals. The resolution of a sensor is the smallest change that it would detect in the measurable quantities (2).

Some sensors could also have an impact on what they measure; for instance, some chemicals react to form a covalent complex with the sensing molecule (3). Often in a digital display, the least significant digit will fluctuate, which it is indicating that some of the magnitude changes would be resolved. The resolution relates to the precisions with the performed measurements. Sensors need to be designed to have a small effect on what is measured. Making the sensors smaller often improves the explained properties and may introduce other advantages. In this study, were investigated the electronic and physicochemical properties of helium adsorption on Ytterium (^{39}Y)-doped BN flake as a sensor for He detection (4,5).

Helium is an inert gas and does not easily combine with other elements. It was used as an inert shield for arc welding, to pressurize the fuel tanks of liquid fueled rockets and in supersonic wind tunnels. Helium gas was applied to inflate blimps, scientific and party balloons (6). A mixture of helium and oxygen was used as an artificial atmosphere for divers and others working under pressure. Different ratios of He and O_2 were used for different diver operation depths (7). Helium has extracted from natural gas. It has been detected spectroscopically in great abundance, especially in the hotter stars, and it is an important component in both the proton–proton reaction and the carbon cycle, which