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Research Article

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A Comparative study of SCN^- adsorption on the $Al_{12}N_{12}$, $Al_{12}P_{12}$, and Siand Ge - doped $Al_{12}N_{12}$ nano-cages to remove from the environment

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ABSTRACT

The geometry, electronic structure, and catalytic properties of $Al_{12}N_{12}$ and $Al_{12}P_{12}$ nano-cages are investigated by density functional theory calculations. The results express that toxic gas SCN^-adsorption upon the Al atom of $Al_{12}N_{12}$ is stronger than that of isolated $Al_{12}P_{12}$ nano-cage. The adsorption value is about −192.74 kJ mol^{-1}, which is reason via the chemisorptions of SCN anion. The computed density of states (DOS) indicates that a notable orbital hybridization take place between SCN^- and $Al_{12}N_{12}$ nano-cage in adsorption process. Finally, the $Al_{12}N_{12}$ nano-cage can be used to design as useful sensor for nanodevice applications.
Hence, we concluded that the Si-doped $Al_{11}N_{12}$ nano-cage can be served as a reliable material for SCN^- adsorption.

1. Introduction

Environmental pollution is one of the most important problems that human beings face and due to the increase in population and the expansion of industries, the importance of controlling environmental pollution and preventing its exponential growth, is felt more than ever. Problems caused by the presence of pollutants that are not biologically eliminated, have led humans to identify different ways to reduce or eliminate them. For a long time, various processes have been implemented to remove harmful environmental pollutants from water, wastewater and air, which have not had a very good efficiency. In recent years, nanotechnology has played a significant role in green chemistry and the use of nanoparticles in the removal of environmental pollutants is considered as one of the newest methods of removing pollutants in the world. These materials have a very good performance in controlling environmental pollution due to their high surface-to-volume ratio and excellent chemical activity and production of harmless products. This article introduces some of the most important nanoparticles and their application in the removal of environmental pollutants.

Thiocyanate is the anion (SCN^-). Due to the high level of the importance of thiocyanate anion detection in both atmospheric and environmental sciences, a wide variety of investigations have been done upon the adsorption of this molecule both theoretically and experimentally [1–11]. SCN^- anion is the product of reaction between CS_2 and NH_2-species and also reaction between $CH_3SCN + e^-$ $SCN^- + CH_3^\bullet$ and it can be found in interstellar ice and dust clouds. Quite fadeaway or reducing SCN^- in human body is highly important regarding the human host defense system. It may happen via biosynthesis of hypothiocyanite by a lactoperoxidase. Moreover, the photoelectron spectrum of thiocyanate anion has been studied reporting the adiabatic electron affinity of SCN^- radical [8,14]. The SCN^- can play notable roles in determining the structure of polymeric transition-metal complexes. The SCN^- anion is a very adaptable ambidentate ligand with two donor atoms [9–13]. In thiocyanates, the organic group (or metal ion) is attached to sulfur: R−S−C≡N has a S-C single bond and a C≡N triple bond [15]. In isothiocyanates, the substituent is attached to nitrogen: R−N=C=S has a S=C double bond and a C=N double bond.

Also The dangerous reaction between thiocyanate anion and acids, it is possible to release highly toxic gases. Nanotechnology can act as a green technology in the destruction and transformation of various environmental pollutants. The most prominent feature of this

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