Identification and sensing of hydrogen fluoride (HF) on aluminum phosphide ($Al_{24}P_{24}$) nanocage in both gas and water phases: electronic study via density-functional theory computations

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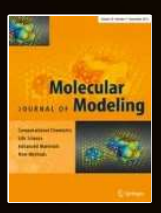

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Aims and scope →

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Abstract

Context

Hydrogen fluoride (HF) is extensively present in environmental and industrial pollutants. It may harm the health of humans and animals. This work evaluated the adsorption of an (HF)*n* linear chain (*n* = 1, 2, 3, and 4) onto an AlP nanocage through ab initio calculations for the evaluation of its performance in sensing and monitoring (HF)*n* within aqueous and gaseous media.

Methods

The present work adopted density functional theory (DFT) at the 6−311 G (d, p) basis set to analyze (HF)*n* linear chain adsorption onto AlP nanocages with the B3LYP functional. This paper examined the adsorption energy, configuration optimization, work function, and charge transfer. In addition, the contributions of the HF linear chain size to electronic properties and adsorption energy were measured. The dimer form of HF on the surface of AlP nanocages was found to have the highest stability based on the adsorption energy values. Once (HF)*n* was adsorbed onto the nanocage, the HOMO–LUMO energy gap experienced a large reduction from 3.87 to 3.03 eV, enhancing electrical conductivity. In addition, AlP nanocages may serve in the sensing of (HF)*n* under multiple environmental pollutants.