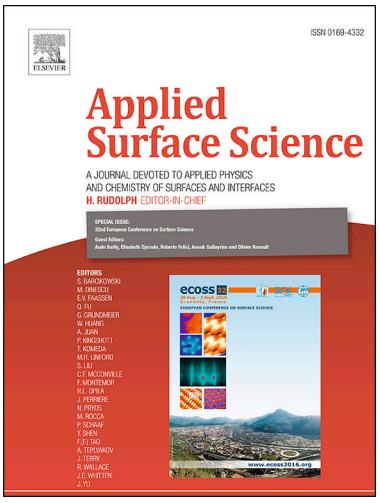

Full Length Article

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Adsorption behavior of COF_2 and CF_4 gas on the MoS_2 monolayer doped with Ni: a first-principles study

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Abstract

CF_4 and COF_2 are the two main decomposition products of fluorocarbon gas insulating medium. We explored the gas sensing properties of Ni-MoS_2 to CF_4 and COF_2 based on the density functional theory calculations. The adsorption energy, charge transfer, density of states and electron density difference have been discussed. It was found that the interaction between COF_2 molecule and Ni-MoS_2 is strong, and the adsorption energy is 0.723 eV. Ni-MoS_2 acts as the electron donor and transfers some electrons to COF_2 molecule during the interaction. The adsorption energy of CF_4 on Ni-MoS_2 is lower than that of COF_2, and the interaction between them belongs to physical adsorption. Ni-MoS_2 has the potential to be used as a gas sensor for COF_2 detection using in the field of gas insulated switchgear on-line monitoring.

Keywords: COF_2, CF_4, Ni-MoS_2 monolayer, adsorption, first-principles calculation

1 Introduction

SF_6, which has been widely used in the power industry, is a strong greenhouse gas with the global warming potential (GWP) up to 23500 and the atmospheric lifetime of 3200 years. [1-3] In recent years, fluorocarbon gases such as CF_3I (Trifluoroiodomethane), c-C_4F_8 (Octafluorocyclobutane) have been the focus of alternative-gas research due to their excellent environmental and insulating properties [4]. In practical engineering applications, CF_3I and c-C_4F_8 may decompose to produce free radicals such as CF_3· and CF_2· in a discharge. These free radicals can react with trace water or oxygen in the devices, producing some decomposition products such as COF_2 and perfluorocarbons [5]. The generation of the decomposition products is closely related to the insulation status of gas insulating medium. And the formation of toxic products, COF_2, not only poses a threat to the safety of maintenance personnel, but also causes corrosion to the inner wall of the equipment. Therefore, it is necessary to monitor the contents of typical decomposition products.

In recent years, two-dimensional (2D) nanosheets have gained numerous attention. In particular, 2D MoS_2 is proved to be a versatile material for a wide variety of applications such as nanoelectronic devices, catalysis as well as gas sensors [6-8]. Recent researches have shown that MoS_2 nanosheets can sensitively sense a number of molecules. *Late et al.* studied the sensing