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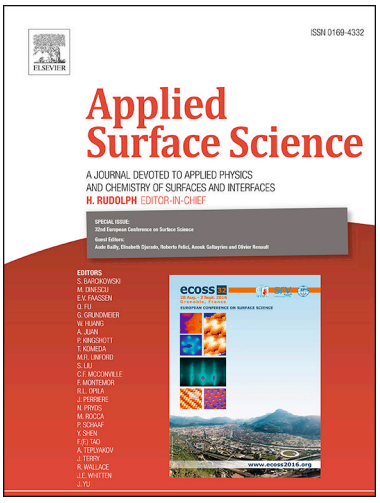

Full Length Article

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Adsorption of phenol and hydrazine upon pristine and X-decorated（X=Sc、Ti、Cr and Mn）MoS_2 Monolayer

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Abstract

Using density functional theory（DFT），we present a theoretical investigation of phenol（C_6H_5OH）and hydrazine（N_2H_4）on pristine and decorated MoS_2 monolayer. In our work，we first focus on the interactions between several metal atoms and MoS_2 monolayer and then choose the MoS_2 nanosheet decorated by Sc、Ti、Cr and Mn to be the substrate. Furthermore，the properties of phenol and N_2H_4 on pure and X-doped（X=Sc、Ti、Cr and Mn）MoS_2 base materials are discussed in terms of adsorption energy，adsorption distance，charge transfer，charge density difference，HOMO and LUMO molecular orbitals and density of states（DOS）. The results predict that the adsorption of phenol and hydrazine upon X-decorated MoS_2 monolayers are more favorable than the adsorption on isolated ones，which demonstrating that Sc、Ti、Cr and Mn doping help to improve the adsorption abilities. Calculations also show shorter adsorption distance and more charge transfer for Sc-、Ti-、Cr- and Mn-doped systems than the pristine one. The results confirm that X-doped MoS_2 monolayer can be used as effective and potential adsorbents for toxic phenol and hydrazine.

Keywords: MoS_2，Metal-decorated，Adsorption energy，DFT，C_6H_5OH and N_2H_4

1. Introduction

Phenol（C_6H_5OH）pollution in the environment mainly means the pollution of phenolic compounds（PCs）in water. The PCs are partially toxic，they will cause acute poisoning or even lead to coma or death when human inhale PCs with high concentrations. So it is necessary to find some effective methods to deal with these compounds. In recent years，a great number of relevant experimental studies have been accomplished[1, 2]，while the theoretical works on toxic substances adsorption or detection were few[3-5]. Due to the limitations of the experimental conditions，we search for a more systematic and effective theoretical approach as an alternative for this problem.

Another toxic agent in waste-water，hydrazine（N_2H_4），occurs naturally as product of microbial nitrogen fixation and has been detected in cigarette smoke. At room temperature，N_2H_4 is a colourless liquid with a penetrating odour. Used as an extraordinary energy material，anhydrous N_2H_4 is extensively applied in nuclear