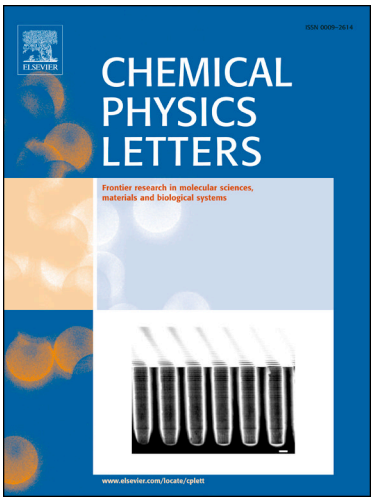

Research paper

Tuning electronic and magnetic properties in monolayer $MoSe_2$ by metal adsorption

Songlei Huang, Quan Zhang, Shuai Liu, Hongping Li, Changsheng Li, Jian Meng, Yi Tian

PII: S0009-2614(17)30837-0
DOI: http://dx.doi.org/10.1016/j.cplett.2017.08.064
Reference: CPLETT 35074

To appear in: *Chemical Physics Letters*

Received Date: 23 July 2017
Revised Date: 24 August 2017
Accepted Date: 30 August 2017

Please cite this article as: S. Huang, Q. Zhang, S. Liu, H. Li, C. Li, J. Meng, Y. Tian, Tuning electronic and magnetic properties in monolayer $MoSe_2$ by metal adsorption, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.08.064

Tuning electronic and magnetic properties in monolayer $MoSe_2$ by metal adsorption

Songlei Huang,[a] Quan Zhang,[a] Shuai Liu,[a] Hongping Li,[a,*] Changsheng Li,[a] Jian Meng,[b] Yi Tian[c,**]

[a]*Institute for Advanced Materials, School of Materials Science and Engineering, Jiangsu University, Zhenjiang, 212013, P. R. China*

[b]*State Key Laboratory of Rare Earth Resources Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, P. R. China*

[c]*Department of Chemistry, National University of Singapore, 3 Science Drive 3, 1175 43, Singapore*

Abstract

We have systematically explored the electronic structures and magnetic properties of metal Pd, Pt, Cu, Ag, Au and Zn adsorbed $MoSe_2$ monolayer by means of first-principles calculations. It reveals that stable chemical adsorption has been formed between the adatoms Pd, Pt, Cu, Ag, Au and $MoSe_2$ monolayer, however, weak physical interaction is found between Zn and $MoSe_2$ monolayer owing to the small adsorption energy. Both the framework structure and electronic property of the metal adsorbed $MoSe_2$ monolayer are slightly tuned by the adatoms. More importantly, magnetic character is introduced in Cu, Ag and Au systems.

Keywords: $MoSe_2$ monolayer; metal adsorption; electronic and magnetic properties; First-principles calculations

1. Introduction

Since the discovery of graphene in 2004, two-dimensional layered materials have inspired a surge of interests [1-3]. Among them, layered transition-metal dichalcogenides (LTMDs) have attracted a great deal of attention owing to their