

# Accepted Manuscript

Research paper

Nonmetal doping induced electronic and magnetic properties in MoSe<sub>2</sub> monolayer

Hongping Li, Songlei Huang, Quan Zhang, Zhipeng Zhu, Changsheng Li, Jian Meng, Yi Tian

PII: S0009-2614(17)31089-8  
DOI: <https://doi.org/10.1016/j.cplett.2017.12.010>  
Reference: CPLETT 35286

To appear in: *Chemical Physics Letters*

Received Date: 12 August 2017  
Accepted Date: 5 December 2017

Please cite this article as: H. Li, S. Huang, Q. Zhang, Z. Zhu, C. Li, J. Meng, Y. Tian, Nonmetal doping induced electronic and magnetic properties in MoSe<sub>2</sub> monolayer, *Chemical Physics Letters* (2017), doi: <https://doi.org/10.1016/j.cplett.2017.12.010>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# Nonmetal doping induced electronic and magnetic properties in

## MoSe<sub>2</sub> monolayer

Hongping Li,<sup>a,\*</sup> Songlei Huang,<sup>a</sup> Quan Zhang,<sup>a</sup> Zhipeng Zhu,<sup>a</sup> Changsheng Li,<sup>a</sup> Jian Meng,<sup>b</sup> Yi Tian<sup>c,\*\*</sup>

<sup>a</sup>*Institute for Advanced Materials, School of Materials Science and Engineering, Jiangsu University, Zhenjiang, 212013, P. R. China*

<sup>b</sup>*State Key Laboratory of Rare Earth Resources Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022, P. R. China*

<sup>c</sup>*Department of Chemistry, National University of Singapore, 3 Science Drive 3, 1175 43, Singapore*

### Abstract

We have systematically investigated the electronic structures and magnetic properties of nonmetal doped MoSe<sub>2</sub> monolayer by using spin-polarized density functional theory calculations. Formation energies reveal that all doped systems are thermodynamically preferred under Mo-rich conditions than Se-rich conditions, and the incorporation of O atom into MoSe<sub>2</sub> monolayer is most favorable. Electronic structure analysis elucidates that Cl, Br and I doped systems exhibit half-metallic properties, while the band gap has been significantly tuned by H, B, C, N, and F doping. More importantly, H, B, N, F, Cl, Br, and I doping can induce pronounced magnetic moments in host MoSe<sub>2</sub> monolayer.

**Keywords:** density functional theory; MoSe<sub>2</sub> monolayer; nonmetals doping; electronic and magnetic properties

### 1. Introduction

Transition metal dichalcogenides (TMDs), belong to the family of layered materials, attract great scientific and technological interest due to their potential

Download English Version:

<https://daneshyari.com/en/article/7838410>

Download Persian Version:

<https://daneshyari.com/article/7838410>

[Daneshyari.com](https://daneshyari.com)