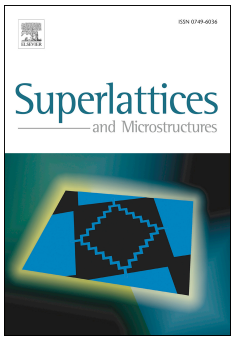
Accepted Manuscript



Effect of structural defects on electronic and magnetic properties of ZrS_2 monolayer

Haiyang Wang, Xu Zhao, Yonghui Gao, Tianxing Wang, Shuyi Wei

PII: S0749-6036(17)33014-8

DOI: 10.1016/j.spmi.2018.02.025

Reference: YSPMI 5517

To appear in: *Superlattices and Microstructures*

Received Date: 24 December 2017

Revised Date: 16 February 2018

Accepted Date: 16 February 2018

Please cite this article as: H. Wang, X. Zhao, Y. Gao, T. Wang, S. Wei, Effect of structural defects on electronic and magnetic properties of ZrS_2 monolayer, *Superlattices and Microstructures* (2018), doi: 10.1016/j.spmi.2018.02.025.

Effect of structural defects on electronic and magnetic properties of ZrS_2 monolayer

Haiyang Wang, Xu Zhao*, Yonghui Gao, Tianxing Wang, Shuyi Wei*

College of Physics and Materials Science, Henan Normal University, Xinxiang, Henan 453007, China

Abstract

We aimed at ten configurations of vacancy defects and used the first-principles methods based on density functional theory to research electronic and magnetic properties of ZrS_2 monolayer. Results show that the system of two-zirconium vacancy(V_{2zr}) and one Zr atom+one S atom vacancy(V_{1Zr+1S}) can induce to total spin magnetic moment of $0.245\mu_B$ and $0.196\mu_B$, respectively. In addition, three and six S atoms vacancy can induce conrresponding system to manifest spin magnetic moment of $0.728\mu_B$ and $3.311\mu_B$, respectively. In S atom vacancy defects, vacancy defects can transform the system from semiconductor to metal, several of the Zr atoms and adjacent S atoms display antiferromagnetism coupling in three apart S atom vacancy defects. Vacancy defects can make the intrisic monolayer ZrS_2 transform semiconductor into metal. These results are important for the achievement of spin devices based on ZrS_2 semiconductor.

Keywords: 2D monolayers; Transition-metal dichalcogenides; vacancy defects

1.Introduction

In recent years, monolayer transition-metal dichalcogenides(TMDCs) have been extensively studied and used, and will be more widely studied in the future. They have great potential applications in some areas, for