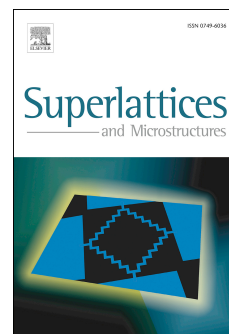


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Effect of structural defects on electronic and magnetic properties of ZrS₂ monolayer

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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 ZrS₂ 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 corresponding 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 intrinsic monolayer ZrS₂ transform semiconductor into metal. These results are important for the achievement of spin devices based on ZrS₂ 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

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