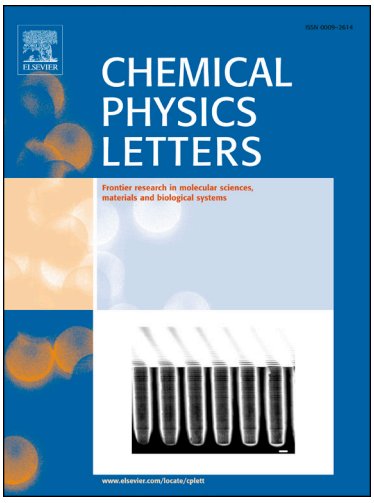

Research paper

Nonmetal doping induced electronic and magnetic properties in $MoSe_2$ monolayer

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Nonmetal doping induced electronic and magnetic properties in $MoSe_2$ monolayer

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Abstract

We have systematically investigated the electronic structures and magnetic properties of nonmetal doped $MoSe_2$ 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 $MoSe_2$ 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 $MoSe_2$ monolayer.

Keywords: density functional theory; $MoSe_2$ 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