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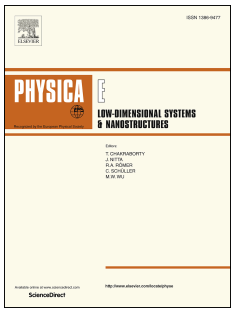

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PII: S1386-9477(17)31987-2

DOI: 10.1016/j.physe.2018.02.013

Reference: PHYSE 13052

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received Date: 27 December 2017

Revised Date: 27 January 2018

Accepted Date: 9 February 2018

Please cite this article as: W.-Z. Xiao, G. Xiao, Q.-Y. Rong, L.-L. Wang, Electronic and magnetic properties of SnS_2 monolayer doped with non-magnetic elements, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.02.013.

Electronic and magnetic properties of SnS_2 monolayer doped with non-magnetic elements

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Abstract:

We performed a systematic study of the electronic structures and magnetic properties of SnS_2 monolayer doped with non-magnetic elements in groups IA, IIA and IIIA based on the first-principles methods. The doped systems exhibit half-metallic and metallic natures depending on the doping elements. The formation of magnetic moment is attributable to the cooperative effect of the Hund's rule coupling and hole concentration. The spin polarization can be stabilized and enhanced through confining the delocalized impurity states by biaxial tensile strain in hole-doped SnS_2 monolayer. Both the double-exchange and *p*-*p* exchange mechanisms are simultaneously responsible for the ferromagnetic ground state in those hole-doped materials. Our results demonstrate that spin polarization can be induced and controlled in SnS_2 monolayers by non-magnetic doping and tensile strain.

Keywords: SnS_2 monolayer; electronic structure; magnetic property; doping; first-principles

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