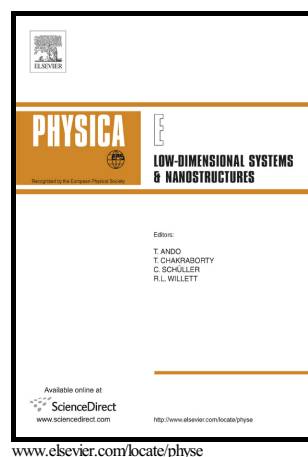


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Tunable electronic behavior in 3d transition metal doped 2H-WSe₂

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Abstract

Structural and electronic properties of 3d transition metal Sc, Ti, Cr and Mn incorporated 2H-WSe₂ have been systematically investigated by first-principles calculations based on density functional theory. The calculated formation energies reveal that all the doped systems are thermodynamically more favorable under Se-rich condition than W-rich condition. The geometry structures almost hold that of the pristine 2H-WSe₂ albeit with slight lattice distortion. More importantly, the electronic properties have been significantly tuned by the dopants, i.e., metal and semimetal behavior has been found in Sc, Ti and Mn-doped 2H-WSe₂, respectively, semiconducting nature with narrowed band gap is expected in Cr-doped case, just as that of the pristine 2H-WSe₂. In particular, magnetic character is realized by incorporation of Mn impurity with a total magnetic moment of 0.96 μ_B . Our results suggest chemical doping is an effective way to precisely tailor the electronic structure of layered transition metal dichalcogenide 2H-WSe₂ for target technological applications.

Keywords: 2H-WSe₂; Metallic impurity; First-principles calculations; Electronic

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