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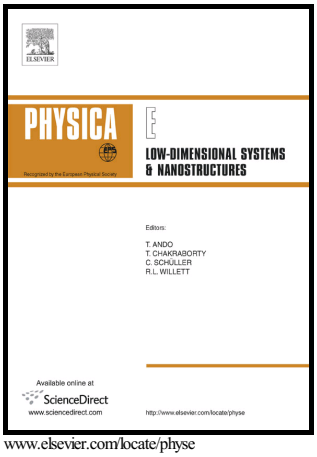

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Tunable electronic behavior in 3d transition metal doped 2*H*-WSe_2

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Abstract

Structural and electronic properties of 3d transition metal Sc, Ti, Cr and Mn incorporated 2*H*-WSe_2 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 2*H*-WSe_2 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 2*H*-WSe_2, respectively, semiconducting nature with narrowed band gap is expected in Cr-doped case, just as that of the pristine 2*H*-WSe_2. 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 2*H*-WSe_2 for target technological applications.

Keywords: 2*H*-WSe_2; Metallic impurity; First-principles calculations; Electronic