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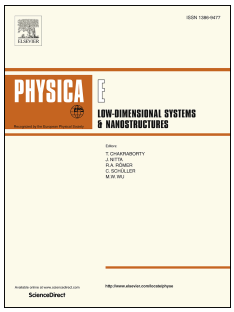

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Magnetic engineering in InSe/black-phosphorus heterostructure by transition-metal-atom Sc-Zn doping in the van der Waals gap

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Abstract

Within the framework of the spin-polarized density-functional theory, we have studied the electronic and magnetic properties of InSe/black-phosphorus (BP) heterostructure doped with 3*d* transition-metal (TM) atoms from Sc to Zn. The calculated binding energies show that TM-atom doping in the van der Waals (vdW) gap of InSe/BP heterostructure is energetically favorable. Our results indicate that magnetic moments are induced in the Sc-, Ti-, V-, Cr-, Mn- and Co-doped InSe/BP heterostructures due to the existence of non-bonding 3*d* electrons. The Ni-, Cu- and Zn-doped InSe/BP heterostructures still show nonmagnetic semiconductor characteristics. Furthermore, in the Fe-doped InSe/BP heterostructure, the half-metal property is found and a high spin polarization of 100% at the Fermi level is achieved. The Cr-doped InSe/BP has the largest magnetic moment of 4.9 μ_B. The Sc-, Ti-, V-, Cr- and Mn-doped InSe/BP heterostructuresexhibit antiferromagnetic ground state. Moreover, the Fe- and Co-doped systems display a weak ferromagnetic and paramagnetic coupling, respectively. Our studies demonstrate that the TM doping in the vdW gap of InSe/BP heterostructure is an effective way to modify its electronic and magnetic properties.

Keywords: InSe/BP heterostructure, Transition-metal-atom doping, Electronic structure, Magnetism, First-principles calculations

1. Introduction

Two-dimensional (2D) materials have shown novel properties and attracted worldwide research interests. As a bright star material, graphene has ultrahigh carrier mobility of 10^5 $cm^2 \cdot V^{-1} \cdot s^{-1}$ [1]. However, the lack of an energy bandgap extremely limits its widespread application because the small