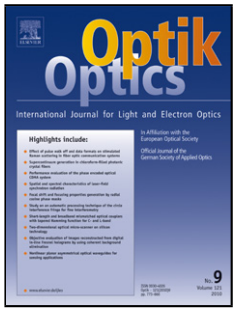

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Tunable magnetism in 2D silicon carbide doped with Co and Fe dopants: Ab initio study

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Abstract

The electronic and magnetic properties of Fe- and Co-doped SiC monolayers are investigated by using first-principles method. The magnetism is observed in both two systems. Particular attention is concentrated on the interaction between Fe-Fe and Co-Co atoms in SiC monolayers. It is found that the magnetic properties switch depending on the TM-TM distance, antiferromagntic (AFM), ferromagnetic (FM) and nonmagnetic (NM) states are found in both systems. With increasing distance between two Co or Fe atoms, the doped SiC monolayer undergoes AFM─FM─NM or FM─AFM─NM transitions, respectively. The results show the *p–d* hybridization mechanism results in its ferromagnetic state. Our studies demonstrate that the Fe- and Co-doped SiC monolayers show tunable electronic and magnetic properties, suitable for applications in electronics and spintronics at nanoscale.

Keywords: SiC; Magnetic properties; First-principles calculation; Tunable magnetism;

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