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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, antiferromagnetic (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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