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Iron and manganese-related magnetic centers in hexagonal silicon carbide: A possible roadmap for spintronic devices

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ABSTRACT

The electronic and magnetic properties of manganese- and iron-doped 4H-SiC were investigated by first-principles calculations, using an all electron methodology. The results on stability, spin configurations, formation and transition energies, local magnetic moments, and hyperfine parameters were compared to available theoretical and experimental data. The results indicated that transition metal impurities are energetically more favorable in lattice sites with carbon atoms as their first nearest neighbors, in both substitutional and interstitial configurations, which results from the larger electronegativity of carbon with respect to that of silicon. The analysis of the electronic properties of those impurity centers showed that they could stay in several stable charge states, depending on the Fermi energy level position within the host SiC bandgap. Additionally, by computing the p-d exchange coupling constant, which is related to a spin polarization in the SiC valence band top, we explored the possibility of achieving macroscopic magnetism in SiC. The results indicated that some centers, in both substitutional and interstitial configurations, present reasonably strong magnetic couplings to mediate macroscopic magnetism at high temperatures, which may generate spin polarized currents, leading to applications in spintronic devices.

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