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Ground-state magnetic properties of transition-metal dopants in silicon carbide[1] WENHAO HU, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — Recently, a decoherence-free subspace(DFS) system has been predicted in the substitutional nickel spin center of diamond [1]. Here we describe our investigations of substitutional transition metal dopants in 3C silicon carbide using density functional theory in the SGGA approximation. We used a 64-atom supercell for the silicon carbide host, inserted a dopant atom (Ni or Cr) at a single carbon or a single silicon site. The atomic positions were allowed to relax with a force precision of 0.1 mRy/a.u. The Heisenberg exchange coupling energy J was calculated as a function of hydrostatic strain. An antiferromagnetic-ferromagnetic transition can be seen in nickel spin centers at certain strains. A model of two spatially separated spins can be used to explain the dependence of J on the atomic separation. By applying a magnetic field, we predict two of the triplet states can be split off so as to create a DFS. Strain modulation and resonant microwave can be exploited to manipulate the qubit. Finally, the experimental feasibility of our scheme is evaluated.

[1] T. Chanier, C. E. Pryor, M. E. Flatté, Europhys. Lett. 99, 67006 (2012)

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