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Substitutional nickel impurities in diamond: decoherence-free subspace for quantum information processing THOMAS CHANIER, CRAIG PRYOR, MICHAEL E. FLATTE', University of Iowa — Magnetic color centers in diamond have received interest as qubits for quantum information processing due to diamond's wide band gap and long spin lifetimes which offer the possibility to initialize, manipulate and readout the quantum state of the qubit. Ni-related impurities have been known to form various color centers in diamond and here we propose the use of a substitutional Ni impurity as a qubit. The electronic and magnetic properties of a neutral substitutional nickel impurity in diamond are studied using density functional theory in the generalized gradient approximation. The spin-one ground state consists of two electrons with parallel spins, one located on the nickel ion in the 3d9 configuration and the other distributed among the nearest-neighbor carbons. The exchange interaction between these spins is due to p-d hybridization and is controllable with compressive hydrostatic or uniaxial strain. For sufficient strain the antiparallel spin configuration becomes the ground state. Hence, the Ni impurity forms a controllable two-electron exchange-coupled system that should be a robust qubit for solid-state quantum information processing.

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