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Theory of single-spin dynamics for transition-metal dopants in diamond[1]

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Spin centers in diamond, especially the well-studied nitrogen-vacancy center, exhibit exceptionally favorable properties for quantum control, including remarkably long room temperature spin coherence times, optical excitation, manipulation by RF fields and optical readout. Although transition-metal dopants in diamond have not been as extensively studied, they offer novel opportunities for external control of single-spin dynamics by comparison, which originate from the symmetry of the dopant's d shell in a tetrahedral lattice and the presence of strong spin-orbit coupling. The d-shell states of a substitutional transition-metal dopant can be either strongly hybridized with the diamond host electronic structure (t2 symmetry states) or very weakly hybridized (e symmetry states) due to a mismatch of the symmetry of the states of the dopant and host. Thus the electronic wave function of the spin-1 ground state of a dopant like Cr is atomic-like and unresponsive to external perturbations of the lattice or an applied electric field. Ni, which also has a spin-1 ground state, has strongly hybridized electronic wave functions and is sensitive to local strain and electric fields. The more extended states that produce the Ni ground state spin provide helpful consequences for spin manipulation. The ground state of Ni is found to behave as a spin-1/2 predominately on the Ni site and a ferromagnetically-oriented spin-1/2 predominately on the four nearest-neighbor carbon sites around the Ni. Under compressive hydrostatic strain the overlap between these two wave functions increases and a transition can be reached where the two spins orient antiferromagnetically; a similar effect is seen in double quantum dots where it has been used to perform exchange-only quantum operations on a qubit composed of the two-electron spin singlet and the zero-magnetization two-electron spin triplet. We propose use of the same effect for strain-mediated control of encoded qubits in diamond.

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