

Abstract Submitted
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Ab initio theory of spin-orbit coupling for quantum bits in diamond exhibiting dynamic Jahn-Teller effect¹ ADAM GALI, GERGŐ THIERING, Wigner Research for Physics, Hungarian Academy of Sciences — Dopants in solids are promising candidates for implementations of quantum bits for quantum computing. In particular, the high-spin negatively charged nitrogen-vacancy defect (NV) in diamond has become a leading contender in solid-state quantum information processing. The initialization and readout of the spin is based on the spin-selective decay of the photo-excited electron to the ground state which is mediated by spin-orbit coupling between excited states and phonons. Generally, the spin-orbit coupling plays a crucial role in the optical spinpolarization and readout of NV quantum bit (qubit) and alike. Strong electron-phonon coupling in dynamic Jahn-Teller (DJT) systems can substantially influence the effective strength of spin-orbit coupling. Here we show by ab initio supercell density functional theory (DFT) calculations that the intrinsic spin-orbit coupling is strongly damped by DJT effect in the triplet excited state that has a consequence on the rate of non-radiative decay. This theory is applied to the ground state of silicon-vacancy (SiV) and germanium-vacancy (GeV) centers in their negatively charged state that can also act like qubits. We show that the intrinsic spin-orbit coupling in SiV and GeV centers is in the 100 GHz region, in contrast to the NV center of 10 GHz region. Our results provide deep insight in the nature of SiV and GeV qubits in diamond.

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