Theory on the optical spin-polarization loop of the nitrogen-vacancy center in diamond

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Dopants in solids are promising candidates for implementations of quantum bits. In particular, the high-spin negatively charged nitrogen-vacancy defect (NV) in diamond has become a leading contender in solid-state quantum information processing[1–4]. 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 states and phonons, i.e. intersystem crossing (ISC). The operation of NV center is based on the ISC processes but still the microscopic theory on these processes has not been fully developed. Understanding the ISC processes might lead to an improved control of NV qubit.

We will show that strong coupling between electrons and phonons in the excited state can naturally explain the observed multiple ISC rates in the excited state branch[5]. Furthermore, we will present a theory including electron-phonon coupling and correlated electron states from *ab initio* calculations that accounts for the optical spinpolarization of NV center and also explains the absorption and photoluminescence spectra of the singlets. Our finding completes the theory of the loop of the optical spinpolarization cycle[6].

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