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Kramers-degenerated Spin Systems “NV+n13C”in Diamond for Quantum Magnetometry: Spin-Hamiltonian and Quantum Chemistry Analysis

Spin properties of single electronic spin of the NV center in diamond coupled to few proximal 13C nuclear spins are studied by spin-Hamiltonian method using available experimental data on hyperfine interactions along with their quantum chemical simulation.

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Summary

Kramers-degenerated Spin Systems “NV+n13C”in Diamond for Quantum Magnetometry: Spin-Hamiltonian and Quantum Chemistry Analysis

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Spin systems consisted of single electronic spin S=1 of the NV center and few nearby isotopic 13C nuclei spins I=1/2 in diamond lattice which can be used as a register of a quantum com-puter [1] or as a sensor of a magnetic field [2] are studied using spin Hamiltonian method. At odd number of 13C nuclei the eigenstates of the spin system at zero external magnetic field are twofold (Kramers) degenerated due to the time reversal invariance of the spin Hamiltonian. This degeneracy is lifted only by external magnetic field regardless of any electric (crystal) field presented thus making such spin systems to be perspective for measurement of a local magnetic field by the NV-based single-spin quantum magnetometer [2].
Here (see also [3]) we have discussed spin properties of such spin systems using experimental data on hyper-fine interactions obtained by observing electron paramagnetic resonance (EPR) on NV ensemble or by moni-toring optically detected magnetic resonance (ODMR) spectra and spin echo modulation on single NV centers. Additionally, we used the density functional theory (DFT) to simulate the H-terminated carbon clusters host-ing NV centers and calculate the hyperfine interaction matrices for 13C nuclei in clusters. We have shown that our cluster simulations provide better correspondence to experimental data even for comparatively small clusters (the largest considered cluster was the C84H78NV cluster) then the super-cell calcula-tions [4] made using much larger super-cells. Moreover, for a first time we have calculated zero-field splitting parameters D and E for the NV center and found for the C84H78NV cluster the values D=2837.23 MHz and E=2.12 MHz.

For the simplest spin system “NV+113C”we got exact analytical expressions for energy levels and eigenstates. Available experimental data [5] on ODMR spectra and spin echo modulation obtained on “NV+n13C”spin cluster are interpreted without fitting parameters.
Additionally, we have studied (see also [6]) the effects of a diamond surface on the NV spin properties depending on position and orientation in the NV center in cluster. The cases of non-passivated as well as H-, OH- and COOH- terminated surfaces (111) are considered. We have calculated hyperfine interaction constants as well as ZFS parameters D and E. All these characteristics have been found to be dependent on position and orientation of the NV center with respect of the surface as well as on the type of surface functionalization. Especially dra-matically spin characteristics are changed (with respect to those for “bulk”clusters) for the NV center near non-passivated diamond surface.

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