



Contribution ID: 92

Type: POSTER

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.

Are you a student, a delegate from developing countries or a participant with physical needs and would like to apply for a sponsored accommodation. Please answer with yes or no.

yes

Please specify whether you would prefer an oral or poster contribution.

poster

Summary

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

A.P. Nizovtsev¹, S.Ya. Kilin¹, A.L. Pushkarchuk², S.A. Kuten³

¹B.I. Stepanov Institute of Physics NASB, Nezavisimosti Ave., 68, 220072 Minsk, Belarus,
e-mail: apniz@ifanbel.bas-net.by

²Institute of Physical Organic Chemistry NASB, Surganova str., 13, 220072 Minsk, Belarus,

³Institute for nuclear problems, BSU, Bobruiskaya str., 11, 220050 Minsk, Belarus

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 computer [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 hyperfine interactions obtained by observing electron paramagnetic resonance (EPR) on NV ensemble or by monitoring 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 hosting 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) than the super-cell calculations [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 dramatically spin characteristics are changed (with respect to those for “bulk” clusters) for the NV center near non-passivated diamond surface.

References

- [1] M.V. Gurudev Dutt et al., Science, 316, 1312 (2007).
- [2] J.R. Maze, et al., Nature, 455, 644 (2008); G. Balasubramanian, et al., Nature, 455, 648 (2008).
- [3] A.P. Nizovtsev, et. al., Optics and Spectroscopy, 108, 230 (2010);
- [4] A. Gali, M. Fyta and E. Kaxiras, Phys. Rev. B, 77, 155206 (2008).
- [5] P. Neumann et al. Science, 320, 1326 (2008).
- [6] V.A. Pushkarchuk, et. al., Optics and Spectroscopy, 108, 254 (2010).

Primary author: Dr NIZOVITSEV, Alexander (Institute of Physics, National Acad. Sci. of Belarus)

Presenter: Dr NIZOVITSEV, Alexander (Institute of Physics, National Acad. Sci. of Belarus)

Track Classification: Semiconductors, Metals and Insulators