Spatial and hyperfine characteristics of SiV^- and SiV^0 color centers in diamond: DFT simulation

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One of the most promising platforms to implement quantum technologies are coupled electron-nuclear spins in diamond in which the electrons of paramagnetic color centers play a role of „fast“ qubits, while nuclear spins of nearby ^{13}C atoms can store quantum information for a very long time due to their exceptionally high isolation from the environment. Essential prerequisite for a high-fidelity spin manipulation in these systems with tailored control pulse sequences is a complete knowledge of hyperfine interactions. Development of this understanding for the negatively charged „silicon-vacancy“ (SiV^-) and neutral (SiV^0) color center, is a primary goal of this article, where we are presenting shortly our recent results of computer simulation of spatial and hyperfine characteristics of these SiV centers in H-terminated cluster $C_{128}[SiV]H_{98}$ along with their comparison with available experimental data.

Keywords: silicon-vacancy (SiV) color center, diamond, ^{13}C nuclear spin, hyperfine interaction, density functional theory.

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