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Negatively-charged NV-center in SiC: Electronic structure properties PRATIBHA DEV, Dept. of Physics and Astronomy, Howard University, Washington, D.C., SOPHIA ECONOMOU, Dept. of Physics, Virginia Tech, Blacksburg, Virginia — Deep defects with high-spin states in semiconductors are promising candidates as solid-state systems for quantum computing applications. The charged NV-center in diamond is the best-known and most-studied defect center, and has proven to be a good proof-of-principle structure for demonstrating the use of such defects in quantum technologies. Increasingly, however, there is an interest in exploring deep defects in alternative semiconductors such as SiC. This is due to the challenges posed by diamond as host material for defects, as well as the attractive properties of SiC. In this density functional theory work, we study the spin-1 structure of the negatively charged NV-center in two polytypes: 3C-SiC and 4H-SiC. The calculated zero phonon line for the excited state of the defect is in telecom range (0.90eV), making it a very good candidate for quantum technologies. This work provides basic ingredients required to understand the physics of this color center at a quantitative and qualitative level. We also design quantum information applications, such as a spin-photon interface and multi-photon entanglement.

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