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Spin states of the silicon vacancy in silicon carbide MICHEL BOCKSTEDTE, University of Salzburg, Austria, and University Erlangen-Nuernberg. Germany, FELIX SCHUETZ, University Erlangen-Nuernberg, Germany — SiC as a semi conductor fulfills all necessary requirements[1] for implementing qubits via defect electron spins, such as the silicon vacancy, the di-vacancy or a complex of a silicon vacancy and a nitrogen impurity. The spin-selective fluorescence in contrast to the prototypical NV-center in diamond operates in the spectral range favorable for telecom applications.Spin-manipulation of the intrinsic centers was demonstrated even at room temperature.[2,3] For the silicon vacancy in SiC inter system crossings (ISCs) from high to yet unknown low spin states govern the spin-relaxation. By DFT and a DFT-based multi-reference Hamiltonian we analyze the spin physics of the defect. In 4H SiC distinct luminescence lines are obtained for the inequivalent defect sites in agreement with experiment. Our result thus establishes an assignment of the lines to the sites. Owing to the spin (S=3/2) and a stronger electron-phonon coupling in the excited state, we find ISCs distinct from the NV-center.

[1] J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2] F. Koehl *et al.*, Nature**479**, 84 (2011).
[3] V. A. Soltamov *et al.*, Phys. Rev. Lett. **108** 226402 (2012).
[4] E. Janzén *et al.* Physica B **404**, 4354 (2009).

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