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Defects as qubits in 3C and 4H polymorphs of SiC[1] LUKE GORDON, AUDRIUS ALKAUSKAS, WILLIAM F. KOEHL, ANDERSON JANOTTI, DAVID D. AWSCHALOM, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Using hybrid functional calculations we study defects in SiC that can serve as qubits for quantum computing. We investigate the divacancy in 4H- and 3C-SiC and the N-V center in 3C-SiC, in which the N impurity replacing a C atom is sitting next to a Si vacancy. The calculated excitation and emission energies of the divacancy in 4H-SiC are in excellent agreement with the available experimental data. Most importantly, we predict that the neutral divacancy and the negatively charged NV center in 3C-SiC have all the required characteristics to serve as qubits; in addition, both defects are stable in n-type 3C-SiC, which is in principle easy to fabricate. We calculate luminescence lineshapes and Huang-Rhys factors for these defects in 4H and 3C-SiC, and compare with experimental photoluminescence spectra.

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