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Quantum computing with defects[1]

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The development of a quantum computer is contingent upon the identification and design of systems for use as qubits, the basic units of quantum information. One of the most promising candidates consists of a defect in diamond known as the nitrogen-vacancy (NV^{-1}) center, since it is an individually-addressable quantum system that can be initialized, manipulated, and measured with high fidelity at room temperature. While the success of the NV^{-1} stems from its nature as a localized "deep-center" point defect, no systematic effort has been made to identify other defects that might behave in a similar way. We provide guidelines for identifying other defect centers with similar properties. We present a list of physical criteria that these centers and their hosts should meet and explain how these requirements can be used in conjunction with electronic structure theory to intelligently sort through candidate systems. To elucidate these points, we compare electronic structure calculations of the NV^{-1} center in diamond with those of several deep centers in 4H silicon carbide (SiC). Using hybrid functionals, we report formation energies, configuration-coordinate diagrams, and defect-level diagrams to compare and contrast the properties of these defects. We find that the $N_C V_{Si}^{-1}$ center in SiC, a structural analog of the NV^{-1} center in diamond, may be a suitable center with very different optical transition energies. We also discuss how the proposed criteria can be translated into guidelines to discover NV analogs in other tetrahedrally coordinated materials.

[1] J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. Van de Walle, and D. D. Awschalom, Proc. Nat. Acad. Sci. **107**, 8513 (2010).

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