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Significance of Accurate Electronic Structure Calculation Methods in Designing Silicon Donor Qubits FAHD MOHIYADDIN, JACEK JAKOWSKI, JINGSONG HUANG, MILTON NANCE ERICSON, CHARLES BRITTON, FRANKLIN CURTIS, EUGENE DUMITRESCU, BOBBY SUMPTER, TRAVIS HUMBLE, Quantum Computing Institute, Oak Ridge National Laboratory — Recent demonstrations of long-lived spin qubits with high control fidelity have enhanced the potential of silicon donors in quantum computing [1]. Verifying the design of prototype silicon qubit devices using computational models provides insight into their electrostatic potential landscape, donor electron wave functions, and spin dynamics [2]. Here, we examine the sensitivity of device verification to the underlying electronic structure model used for the donor. Within the context of a computational workflow, we observe a significant discrepancy in the amplitude of the donor wave function computed using density-functional theory versus tight-binding methods for the case of doped silicon nanocrystals. While both methods can be used to match experimental values for the hyperfine coupling, differences in the calculated electronic amplitude at the donor site suggest that more complicated interactions, e.g., electron-exchange, may become unreliable. Hence, an accurate understanding of the donor wave function in the donor vicinity is critical to device design, as it serves as a handle to vital parameters in donor based quantum computer architectures. [1] J. T. Muhonen et al., Nature Nanotechnology 9, 986-991(2014). [2] T. S. Humble et al., Nanotechnology 27, 42(2016).

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