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Electronic structure of sub-surface Boron acceptors in silicon for potential qubits RAJIB RAHMAN, Purdue University, West Lafayette, IN 47906, USA, JAN MOL, University of New South Wales, Sydney 2052, Australia, GERHARD KLIMECK, Purdue University, West Lafayette, IN 47906, USA, SVEN ROGGE, University of New South Wales, Sydney 2052, Australia — Single acceptors in silicon are investigated as potential qubits. Due to the p-type nature of the valence band (VB), the acceptor states are less susceptible to the hyperfine interaction of the neighboring nuclear spins. The presence of a stronger spin-orbit coupling in the VB also enables the possibility of an all-electric qubit control. Whereas donor qubits exhibit exchange oscillation with separation distance due to conduction band valleys, Boron acceptors are expected to have smoother exchange curves. We investigate the electronic structure of single Boron acceptors in silicon in the presence of electric field, strain, magnetic field, and interfaces. Bulk Boron acceptors have a four-fold degenerate ground state 45 meV above the VB with angular momentum states of 3/2 and 1/2. An interface splits this manifold into Kramer's doublets. Application of E and B fields allow several possibilities for forming a two-level qubit driven by an ac electric field. We compare calculations from atomistic tight-binding theory to scanning tunneling microscope (STM) measurements and k.p calculations. The tight-binding method captures additional wavefunction symmetries due to the crystal that help to explain the STM measurements.

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