Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Phonon induced two-electron relaxation in two donor qubits in silicon YULING HSUEH, ARCHANA TANKASALA, YU WANG, GERHARD KLIMECK, Purdue University, MICHELLE SIMMONS, University of New South Wales, RAJIB RAHMAN, Purdue University — An atomistic method of calculating two-electron spin-lattice relaxation times (T_1) is presented for two donor qubits in silicon. The singlet-triplet two-electron states are calculated from full-configuration interaction (FCI) method with one-electron basis states obtained from the tight-binding Hamiltonian including spin-orbit interaction. The FCI solution enables the investigation of various regimes of donor separations, including very closely separated donor pairs in which rearrangement of excited bonding and anti-bonding states change the wavefunction symmetries. Hyperfine mixing from the nuclear spins is included perturbatively into the two-electron states. To calculate the T_1 times, the electron-phonon Hamiltonian is evaluated from the strain-dependent tight-binding Hamiltonian. The results show how the T_1 times in donor qubits vary with magnetic field and donor separation for each of the three triplets. Moreover, the variation of T_1 with the electric field controlled exchange coupling is also investigated.

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Date submitted: 06 Nov 2015 Electronic form version 1.4