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Phonon induced spin relaxation times of single donors and donor clusters in silicon YULING HSUEH, Purdue University, HOLGER BUCH, University of New South Wales, LLOYD HOLLENBERG, University of Melbourne, MICHELLE SIMMONS, University of New South Wales, GERHARD KLIMECK, RAJIB RAHMAN, Purdue University — The phonon induced relaxation times (T1) of electron spins bound to single phosphorous (P) donors and P donor clusters in silicon is computed using the atomistic tight-binding method. The electron-phonon Hamiltonian is directly computed from the strain dependent tight-binding Hamiltonian, and the relaxation time is computed from Fermi's Golden Rule using the donor states and the electron-phonon Hamiltonian. The self-consistent Hartree method is used to compute the multi-electron wavefunctions in donor clusters. The method takes into account the full band structure of silicon including the spin-orbit interaction, and captures both valley repopulation and single valley g-factor shifts in a unified framework. The single donor relaxation rate varies proportionally to B^5, and is of the order of seconds at B=2T, both in good agreement with experimental single donor data (A. Morello et. al., Nature 467, 687 (2010)). T1 calculations in donor clusters show variations for different electron numbers and donor numbers and locations. The computed T1 in a 4P:5e donor cluster match well with a scanning tunneling microscope patterned P donor cluster (H. Buch et. al., Nature Communications 4, 2017 (2013)).

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