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Atomistic simulations of negatively charged donor states probed in STM experiments ARCHANA TANKASALA, Purdue University, USA, JOE SALFI, SVEN ROGGE, CQCCT, University of New South Wales, Australia, GERHARD KLIMECK, RAJIB RAHMAN, Purdue University, USA — A single donor in silicon binding two electrons (D^-) is important for electron spin readout and two-qubit operations in a donor based silicon (Si) quantum computer, and has recently been probed in Scanning Tunneling Microscope (STM) experiments for sub-surface dopants. In this work, atomistic configuration interaction technique is used to compute the two-electron states of the donor taking into account the geometry of the STM-vacuum-silicon-reservoir device. While 45 meV charging energy is obtained for D^- in bulk Si, the electrostatics of the device reduces the charging energy to 30 meVs. It is also shown that the reduced charging energy enables spin triplet states to be bound to the donor. The exchange splitting between the singlet and triplet states can be tuned by an external electric field. The computed wavefunctions of the D^- state helps to understand how the contribution of the momentum space valley states change with donor depth and electric field.

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