Atomistic modeling of STM patterned donor devices for Si quantum computing

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INTRODUCTION

Quantum computing with doped silicon has attracted vast attention in recent times due to the promise of extremely long spin coherence, and the already existing industrial infrastructure for silicon device fabrication. The ability to place a single dopant in silicon with 1 nm precision has been realized recently by scanning-tunneling microscope (STM) technology, leading to a series of exotic devices, such as a single-atom transistor [1], world's thinnest nanowire [2], and single spin read-out devices [3]. In this method, dense clusters of phosphorus impurities are placed on a plane inside silicon to form various functional units, such as quantum dots, metallic leads, and gates. Based on the atomistic tight-binding method, we have developed models of STM patterned donor clusters, and computed various spin and charge properties relevant to quantum computing. In particular, we compute spin relaxation times (T_1), hyperfine resonance frequencies, and binding energies of donor electrons – all crucial parameters to characterize and control spin qubits.

MODEL

The few impurity clusters (Fig. 1) are modeled by the atomistic tight-binding (TB) method with a 20 band sp3d5s* spin resolved nearest neighbor model. Each donor is modeled by a Coulomb potential screened by the dielectric constant of silicon, with on-site energy corrections to take into account central-cell effects [4]. The model reproduces the full donor spectrum including correct wavefunction symmetries compared to spectroscopic and spin resonance data. Multi-electron occupation energies and wavefunctions are computed using a self-consistent Hartee method with local density approximation to capture exchange and correlation effects. The full TB Hamiltonain of 1.4 million atoms including electric and magnetic fields is solved by a parallel block Lanczos method to obtain the lowest few donor bound states below the conduction band. Phonon induced spin relaxation rates are computed by evaluating the electron-phonon Hamiltonian in the basis of the donor wavefunctions using the deformed crystal Hamiltonain. Hyperfine resonance frequencies are computed from the wavefunction densities at the nuclear spin sites.

DISCUSSION

Fig. 2 shows the T_1 times of single and few donor clusters in silicon with different electron occupation as a function of B-field. The rate is found to vary as B^5, and yields a T_1 of 1s at 1.5 T for a bulk donor, in close agreement with experiments [3], [5]. The T_1 times depend on multiple conduction valley occupation and spin-orbit interaction, and a full band description is necessary to obtain correct magnitudes and trends. Fig. 3 shows the hyperfine spin resonance frequencies of a 4-donor single electron cluster. Such spin level information is used in electron spin resonance experiments to manipulate and control spin qubits. Fig. 4 shows the binding energies (BE) of different electrons bound to 1P, 2P, and 3P clusters. The BE decreases with electron number as the nuclear positive charges are screened by the electrons.

CONCLUSION

The atomistic modeling of donor clusters helps to understand experimental measurements, and also to design and characterize silicon qubits.

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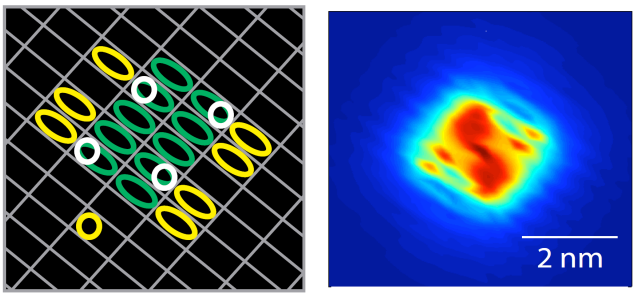

Fig. 1. Schematic (dimer representation) and wavefunction of a four donor cluster in silicon.

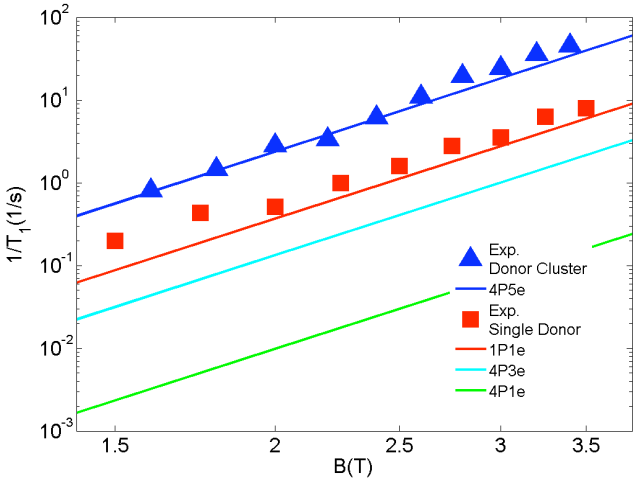

Fig. 2. Spin relaxation times of a bulk donor and a donor cluster in silicon as a function of B-field.

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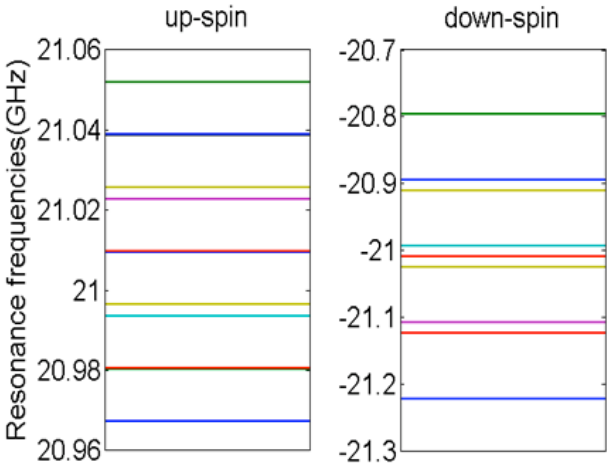

Fig. 3. Hyperfine resonance frequencies of a donor cluster relative to a phosphorus donor ground state energy of -45.6 meV.

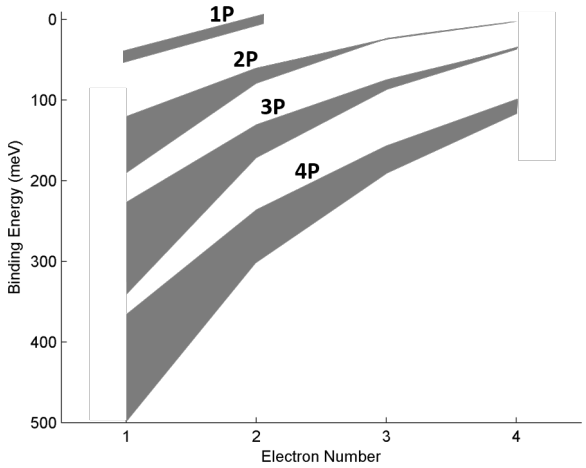

Fig. 4. Binding energies of the first few electrons in a donor cluster.