Quantum Confinement of Donor Molecule Systems in Silicon

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Atomically controlled phosphorus doping in silicon has proven to be a promising candidate for scalable quantum computing architecture[1]. Understanding of the electron confinement in single and multiple donor quantum dots is crucial for control and manipulation of qubits[2]. In this work, we apply a comprehensive 20-band $sp^3d^5s^*$ tight-binding model with self-consistent field Hartree method to calculate energies of multi-electron states. This method enables us to investigate the charging energy of quantum dots consisting of two donors for various orientations in a sub-3nm regime. The two donor quantum dots act as molecular systems with Bohr radius linearly dependent on the separation. Following the inverse relation of the energy states of hydrogenic systems on the Bohr-radius, we find an inverse dependence of the charging energies on the donor separation modulated by valley interference effects. As more electrons are loaded onto the dots the screening effect from inner electrons makes the charging energy weakly dependent on the exact donor locations. This work can serve as a non-invasive metrology to determine the donor locations in such donor dots.

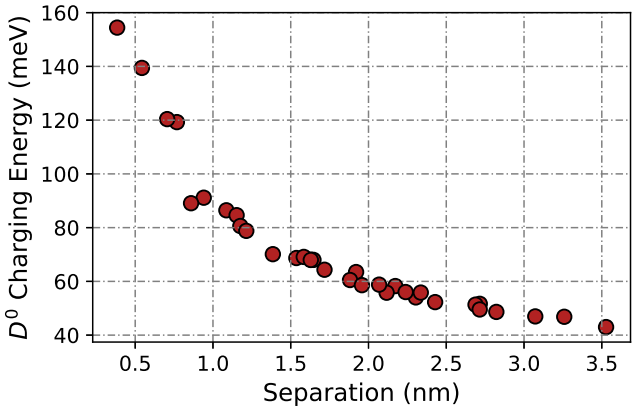

Figure 1: Charging energy of two donor system for one electron to two electron transition with separation.

[1] He, Yu, et al. "A two-qubit gate between phosphorus donor electrons in silicon." Nature 571.7765 (2019): 371-375.

[2] Wang, Yu, et al. "Highly tunable exchange in donor qubits in silicon." npj Quantum Information 2.1 (2016): 1-5.