Ab-initio study of electronic and transport properties of single- and co-doped silicon nanostructures

Mizuta Lab, 1140210, Le The Anh

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Recently, single dopant electronics has opened a new group of extremely-small and low power devices, including single-electron FETs. The basic operations of single dopant devices are based on single-electron tunneling mediated by a single dopant. The binding energy of donor electrons should be much higher than the thermal energy to ensure single dopant devices operate at room temperature; therefore, it is important to accurately estimate the binding energy of donor electrons not only for single dopant devices in particular, but also for nanometer-scale devices in general. In bulk silicon, the donor ground state is shallow and independent from the bottom of the conduction band of Si crystal. In nano silicon, which has dimensions smaller than the Bohr radius of donor electrons in bulk, the interaction between the donor related states and the host Si conduction states becomes significant due to the strong nanoscale confinement. The binding energy in nano Si therefore should be studied from a different point of view to the binding energy in bulk Si.

By performing DFT calculations, I have determined the binding energy of electrons bound to a single phosphorus donor atom in silicon nanorods. The projected density of states (PDOS) and 3D wavefunctions (3DWFs) analysis can clarify the gradually decreasing contribution of the phosphorus electron states from the donor ground states to the higher energy donor excited states due to the hybridization of the donor electron states and silicon electron states. Therefore, I can identify the energy of the first conductive state. The binding energy of the donor electrons in the single P-doped Si nanorods, which have an average radius smaller than 1.4 nm (which is smaller than a_0 = 3nm, the Bohr radius for phosphorus electrons in bulk Si) is calculated as the difference between the first conductive state and the donor ground state. I have found that the binding energy is still around 1.5 eV. As the size decreases below 1.4 nm, the first conductive state is capped near the top of the atomistic effective potential at the phosphorus donor site, whereas above the potential top the electron wavefunctions are more delocalized and can attribute to conduction. This causes the binding energy in sub-1.4 nm Si nanorods to be weakly dependent on the sizes. This fact signifies the good tolerance level of the binding energy, which governs the operating temperature of single dopant-based transistors in practice. The transmission spectra calculated by the non-equilibrium Green's function, which reflects into the transport properties of electrons in silicon nanorod devices, show consistent results with the PDOS-3DWFs method, proving the validity of the new method.

Following this, I have applied the PDOS-3DWFs method to investigate the dependence of binding energy on the position of P atoms in single P-doped cross-shaped Si nanotructures. When the P atom is located at the wing of the cross-shaped nano structure, it is more difficult for the wavefunction to spread entirely within the structure, especially along the horizontal transport direction; this results in higher binding energy for the P atom at the wing of the cross-shaped Si nanostructure. The experimental study of stub-channel FETs, which is similar to cross-shaped model established by the Tabe group from Shizuoka University, shows that electron tunneling has higher barrier energy than conventional straight shape FETs. The theoretical results of the cross-shaped Si nanostructures are consistent with the experimental results for the stub-channel FETs.

Finally, the interaction between donor D^0 and acceptor A^0 ground states have been studied theoretically in phosphorus-boron co-doped silicon nanorods; the different effective atomistic potential at the P site and B site decreases from about 1.5 eV to around 0.5 eV when the two dopants move closer towards each other from 2.17 nm to 0.23 nm. This suggests that the built-in atomistic potential in co-doped silicon nanorods strongly depends on the P-B separation. Moreover, the D^0 wavefunction is destructive at the boron site, whereas the A^0 wavefunction is destructive at the phosphorus site. When two dopants come closer, the overlapping of the B and P original atomic orbitals increases. As a result, the values of wavefunctions of A0 and D0 at the boron and phosphorus sites decrease. The wavefunctions become less localized and shallower, which is consistent with the transmission analysis that transmissions associated with dopant induced states change in nature from discrete to continuous.