First-principle calculations of the interactions between single phosphorus donor and boron acceptor in the P-B co-doped silicon nanostructures

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Recently, the co-doping of Si nanocrystals with P and B has been studied intensively with the aim of utilizing the unique structural properties of Si nanocrystals [1-3]. In past studies [2, 3], we discussed briefly how the donor and acceptor ground states were formed in the P-B co-doped Si nanostructures. The donor ground states were dominated by s-orbitals, while the acceptor ground states were dominated by p-orbitals [3]. The original nature of the donor and acceptor ground states were preserved, even when P and B are close to each other at distances below 1 nm [2]. In this study, we systematically investigate the interactions between single phosphorus donor and boron acceptor by gradually changing the P-B distance from 2.17 nm to 0.23 nm. We found that when two dopants are moved to the nearest neighbor sites, the A0 and D0 wavefunctions become more distorted and less localized. The top-most wavefunction in Fig. 1(a) shows that D0 donor ground state of single P-doped nanorod is constructive at the P site compared to the LUMO state of the undoped Si structure in Fig 1(b). Compared to the HOMO state of the undoped structure in Fig. 1(b), the bottom-most wavefunction of the A0 acceptor ground state of the single B-doped nanorod in Fig 1(c) is constructive at the B site. Compared to the HOMO state of the undoped structure, the D1 state of the single P-doped nanorod is destructive at the P site. As a result, the A0 wavefunction has a small magnitude or is destructive at the P site (Fig 1(d)). Similarly, the D0 state is destructive at the B site, as can be seen in Fig. 1(d). Such destructive interference results the A0 and D0 states to become delocalized and shallower. The delocalized wavefunctions support the transport via the A0 and D0 ground states, thus the transmission rates via the A0 and D0 states increase. Such enhancement suggests the possibility of utilizing electron tunneling via A0 and D0 ground states in the nanoscale p-n junction. Co-dopant position dependence of the atomistic built-in potential will also be discussed in the presentation. The research was partially supported by the Grants-in-Aid for Scientific Research (KAKENHI No. 23226009, 25630144).