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Ab-initio study of interactive-donor states of multiple P-atoms in Si nanoplates

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Individual and coupled dopant atoms in silicon nanodevices play important roles in the transport characteristics [1-4]. In the previous talk [5], we discussed the *ab-initio* study of the donor electronic states of Si nanostructures containing only one P donor. The donor ground state was found at the Fermi level with s-like symmetry. We also studied the projected density of states of single and two P donors in Si nanorods [6] and it was found that two donor states couple together and form the bonding and anti-bonding states.

For understanding the properties arising from strong coupling of multiple donors in nanoscale, we address, in this study, the analysis of the electronic states of Si nanoplates containing several P donors with varying coupling. Figures 1(a) and 1(b) show in the upper panels the configurations of Si nanoplates, NP1 and NP2, with the same dimensions, but containing three P donors closer to each other in the case of NP2. The wavefunctions for the donor states are shown in the lower panels for each case. These states correspond to the density-of-states (DOS) peaks marked in Fig. 1(c). Wavefunctions (I), (II), and (III), corresponding to the case of more isolated P donors, NP1, are strongly localized at the P positions with s-like symmetry. On the other hand, the wavefunctions (IV) and (V), corresponding to the closely packed P donors, NP2, spread within the area of the three P donors, especially for the wavefunction (IV).

These findings provide insights into the effects of the interaction between closely-packed donors, offering a possibility to design functions using multiple P donors with variable coupling strengths.

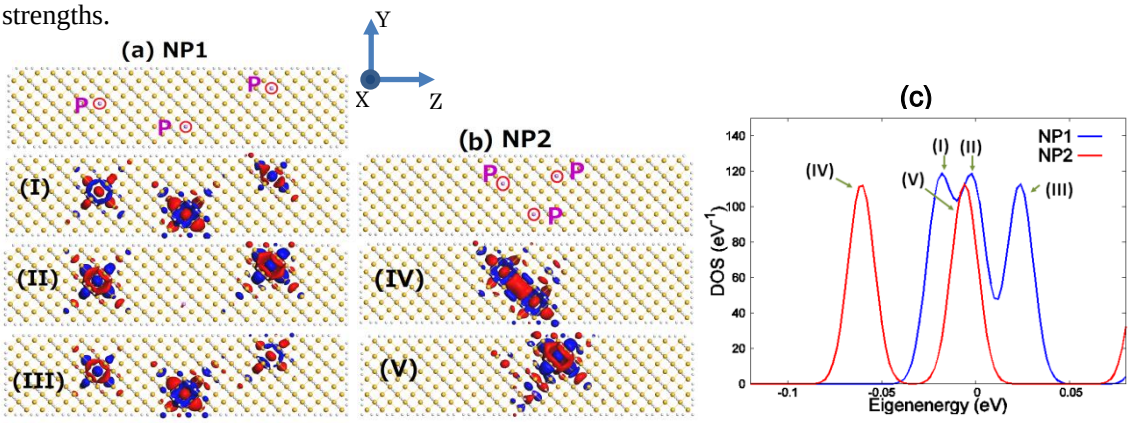

Fig. 1. (a) and (b) Top views of nanoplates, NP1 and NP2, containing three P donors and 3D wavefunctions (I)-(V). (c) Corresponding DOS peaks (I)-(V) near the conduction band edge.

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