単一ドーパントシミュレーション

－ ナノ構造内ドーパント原子の状態と電子輸送 －

Ab initio simulation of single dopant devices: electronic states and transport

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Ab initio approach becomes essential in analyzing discrete dopants in extremely-scaled silicon nanodevices as the random configuration of dopants significantly influences the overall device characteristics. The individual dopant atoms are expected to show fairly different properties compared to those in bulk silicon due both to quantum and dielectric confinement in the silicon nanostructures. We adopt a fully atomistic simulation, Atomistic Toolkit ATK-DFT 10.8, which combines the calculation of electronic states using density functional theory (DFT) with transport calculations based on the non-equilibrium Green's Function (NEGF) method. We study the variability of electronic and transport properties of silicon nanorod transistors with single and a few dopant atoms [1].

In the presentation, we first overview *ab initio* studies of ***isolated*** silicon clusters with discrete dopants reported in the past [2]-[4] in terms of formation energy and ionization energy. We then discuss our recent studies on the impact of location of a single phosphorus dopant in silicon nanorods ***with contacts*** relative to the surface and edge of the nanorod, as well as relative to the metal electrodes.

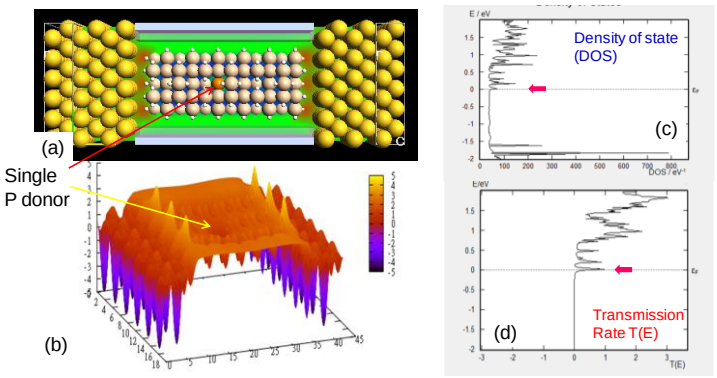

Fig. 1. (a) A Si nanorod transistor, (b) atomistic potential distribution, (c) density of state and (d) transmission spectra.

The electronic properties of a single dopant placed in the vicinity of the source and drain electrodes are of particular interest for investigating the screening effects of metallic electrodes on the dopant potential [5]. We also discuss the dependence of the stability, electronic properties and electrical characteristics of the nanorod transistors on the number and configuration of a few dopants.

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