Computational Modeling of Short Circuit Current in Doped Silicon Nanowires

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Silicon nanowires (SiNWs) are one of the most important semiconductor nanowires and have attracted many attentions because of their extraordinary properties.[1] Doping provides additional functionalization and wider range of useful properties to fully use SiNWs. A p-n junction can be formed by the close contact of n-type doped silicon and p-type doped silicon. Vapor-liquid-solid (VLS) mechanism[2] to grow SiNWs uses gold as the metallic catalyst, leading to gold contamination. This study presents an ab initio analysis of the SiNW composed of gold clusters linked to aluminum and phosphor co-doped silicon quantum dots (QDs) along [111] direction. The density functional theory (DFT) is used to compute the electronic structure of the simulated system. Nonadiabatic coupling implemented in the form of dissipative equation of motion for reduced density matrix is used to study the phonon-induced relaxation in the simulated system.[3] The density of states clearly shows that the formation of Au-Si bonds influences the band gap of co-doped Si. In addition, simulated results show that the electron is promoted from aluminum to phosphor in the photon-mediated process and then recombines to the ground state through golden bridge. This simulation illustrates the basic effect of a photovoltaic cell in the limit of short current circuit.

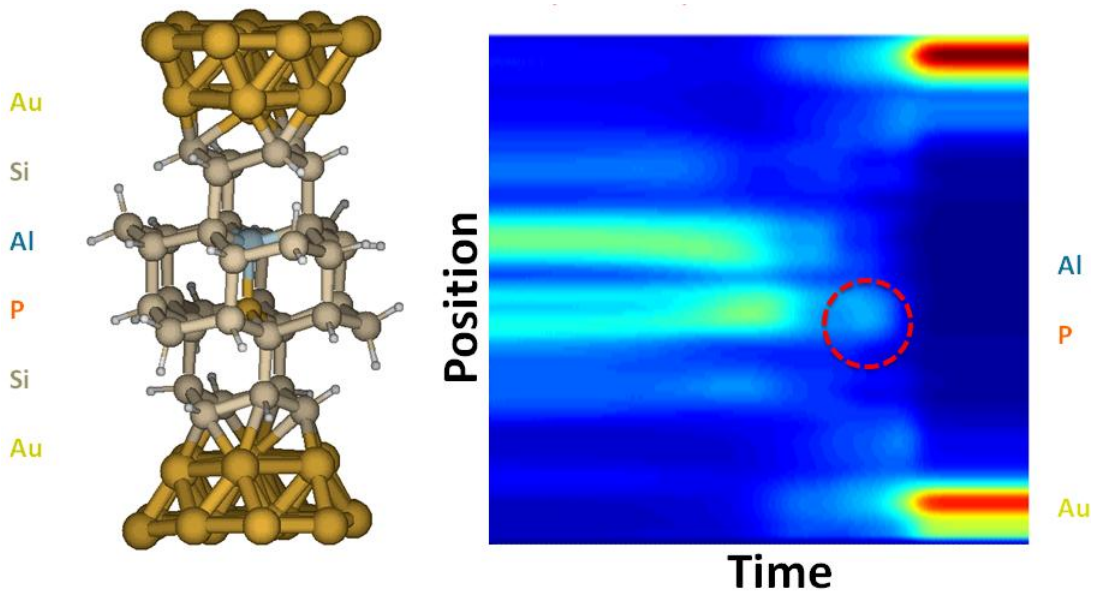

Figure 1, left: optimized geometry of the simulated system, right: time evolution of nonequilibrium electron density in conduction band. Electron reaches bottom terminal earlier (red circle).

1. Hochbaum, A. I.; Yang, P. D., Semiconductor Nanowires for Energy Conversion. *Chem Rev* **2010,** *110* (1), 527-546.
2. Wagner, R. S.; Ellis, W. C., VAPOR-LIQUID-SOLID MECHANISM OF SINGLE CRYSTAL GROWTH. *Applied Physics Letters* **1964,** *4* (5), 89-90.
3. Chen, J.; Schmitz, A.; Kilin, D. S., Computational simulation of the p-n doped silicon quantum dot. *International Journal of Quantum Chemistry* **2012,** *112* (24), 3879-3888.