Structural and Optoelectronic Properties of Silicon Nano-Hetero-Junctions

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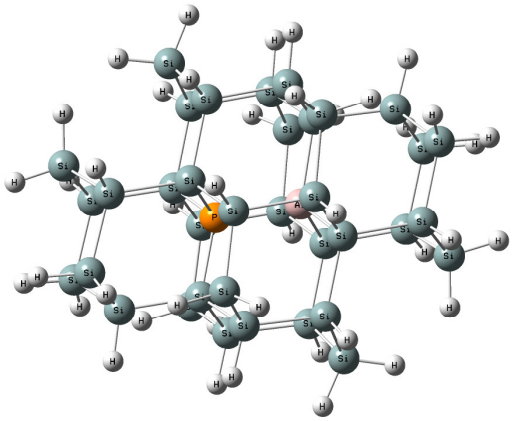

Doped silicon nanostructures are promising materials for electronics and photonics, in particular for applications to solar energy transformation. In this contribution, we computationally study a minimal-size silicon quantum dot elongated in <111> direction with aspect ratio 4:3, doped simultaneously with both n- and p-types of dopes. Thus we consider $Si_{36}H_{42}Al\,P$ as well as $Si_{37}H_{42}P$ and $Si_{37}H_{42}Al$ in comparison with the pure silicon $Si_{38}H_{42}$ elongated quantum dot. We explore structural and optoelectronic properties of this model using DFT-based methods.

Binding/implantation energy is computed for various placements of dopings inside and on the surface of the model. We also simulate dynamics of the quantum dots at various vibration temperatures. Starting from some temperature, one expects to observe the Czochralski effect of Si-monocrystal purification, which is a dope ousting from the crystal to its surface. This simulation demonstrates possible mechanisms of ousting of the dopes. The transition states and corresponding activation energies for possible branches of the reaction of purification are found. That provides information on how fast and in what proportion the dopes are ousted to the surface. Our simulation predicts probability of appearance of bonded pair Al-P on the model surface.

Using TD-DFT we predict linear and two-photon absorption spectra and radiative lifetime for the lowest singlet excited states. We obtain the measure of charge transfer for the excited states – their permanent electric dipole moments. We compare the TD-DFT and ΔSCF methods in calculation of the band gap and the permanent dipole. The latter was employed for geometry optimization and estimation of non-radiative lifetime of the lowest singlet excited state.

Our computation follows basic trends brought by a combined effect of doping and anisotropic quantum confinement on photoexcited charge transfer in silicon nanostructures.

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