First-Principles Study of Electron Dynamics with Explicit Treatment of Momentum Dispersion on Si Nanowires along Different Directions

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In this research, electron dynamics along with ground state structure and optical properties of Si nanowires oriented in various directions are reviewed. These wires can be most significant functional units of future nanoelectronic devices. All observables are computed for a distribution of wave vector[1] at ambient temperatures. Optical properties are computed under assumption of momentum conservation $\Delta\vec{k} = 0$. Under this approximation, the total absorption spectrum is composed of partial contributions to absorption from fixed values of momentum, $a_{tot}(\omega) = \frac{1}{N}\sum_{\vec{k}} a_{\vec{k}}(\hbar\omega)$ with N being normalization. Partial contributions include sum over inter-band transitions $a_{\vec{k}}(\hbar\omega) = \Sigma_{i\in CB}\Sigma_{j\in VB} f_{ij,\vec{k}}\delta\left(\hbar\omega - \hbar\omega_{ij,\vec{k}}\right)$ at a given value of momentum $\vec{k}$, where $\hbar\omega_{ij,\vec{k}} = \varepsilon_j(\vec{k}) - \varepsilon_i(\vec{k})$. The on-the-fly non-adiabatic couplings for electronic degrees of freedom are obtained along the *ab initio* molecular dynamics nuclear trajectories.[2] These couplings are used as parameters for Redfield density matrix equation of motion, which helps to explore the photo-induced processes in these.[3] The main outcomes of this study are transition energies, light absorption spectra, electron and hole relaxation rates, and electron transportation properties. The results of these calculations would contribute to the understanding of the mechanism of electron transfer process on the Si nanowires.

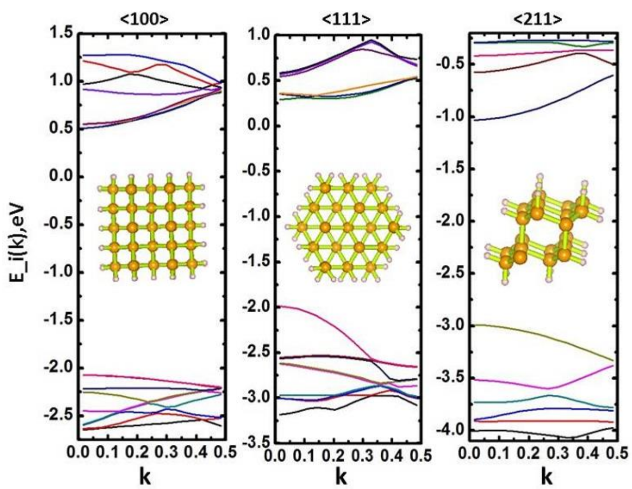

Figure 1: Computed dispersion curves for periodic silicon nanowires grown in <100>, <111>, and <211> crystallographic directions shown as function of dimensionless wavevector. <100> and <211> nanowires show direct bandgap at gamma point. The <111> nanowire shows conduction band with minimum near k/a=0.25, related to indirect gap.

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