FIRST-PRINCIPLES INVESTIGATION OF THE ELECTRONIC, VIBRATIONAL, AND OPTICAL PROPERTIES OF SILICON NANOWIRES*

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Semiconductor nanowires have potential applications in many fields such as optoelectronics, photovoltaic cells, and especially device miniaturization. We have performed calculations of the electronic, vibrational, and optical properties of silicon nanowires using first-principles approaches. Structure relaxation and lattice vibrations are studied within the framework of the density functional theory. The quasi-particle spectra are evaluated using the many-body perturbation theory with the GW approximation. Excitonic effects are included by solving the Bethe-Salpeter equation.

We have studied the structural, electronic, and optical properties of hydrogen-passivated silicon nanowires along [110] and [111] directions with a diameter up to 4.2 nm. The size and orientation dependence of the band gap is investigated. Quantum confinement becomes significant for $d < 2.2$ nm, where new low-energy absorption peaks start to appear in the imaginary part of the dielectric function for polarization along the wire axis [1].

We further investigated the lattice vibrations for silicon nanowires along the [110] direction and the distribution of phonon modes at the Gamma point for nanowires of various diameters. Two different frequency shifts are found for the optical modes and the collective modes, respectively. When the size of nanowires decreases, the frequencies of optical modes are red-shifted, while the frequencies of collective modes are blue-shifted. We provide an explanation for these trends based on different quantum confinement effects. In addition, the controversy over clamped and free boundary conditions is resolved in light of our first-principles calculations. The relative Raman scattering activity and its size-dependence in a small nanowire are evaluated. We also find that quantum confinement considerably changes the sound velocity, which has a significant effect in the studies of transport properties in nanostructures.

Finally, we report the effect of electron-hole interaction on the optical spectra. Due to quantum confinement and reduced screening, a large exciton binding energy of the order of 1 eV is found. The excitonic effect also creates some strong absorption peaks in silicon nanowires.

*In collaboration with C. M. Wei, X. Zhao, L. Yang, C. D. Spataru, and S.G. Louie.

[1] X. Zhao, C. M. Wei, L. Yang, and M. Y. Chou, Phys. Rev. Lett. 92, 236805 (2004).