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Electron structure of silicon nanowires matrix from ab initio calculatious

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The study of quantum-dimensional structures based on Si, Si nanowire particularly attracted attention in connection with the hope to create for optoelectronic devices based on them. This control optical properties of such devices can be controlled, for example, the size (diameter) nanowire, distance between them that determines the degree of porosity) and foreign body behavior of atoms in our systems.

One of the most powerful theoretical approaches to the study of a given structure of nanocrystals are self-consistent calculation using equations formulated in the work of Kohn and Sham.

Facilities such calculations developed a number of software packages using the distributed multiprocessor computing powered by MPI and CUDA.

In the calculations assumed the following type nanocrystalline interface: all dangling bonds on the border nanowire saturated with hydrogen, and the nanocrystals is in a vacuum. This leads to the formation of electrons potential konfaynementu that prevented the carrier out of the nanocrystals.

For comparison of calculated spectra of bulk crystal. Applied software package implements the solution of the Kohn-Sham in the basis of linearized plane waves associated with the corresponding step in grid A.

Convergence of self-consistent cycle determined by the difference between the full energy systems that met two successive stages of the cycle eV.

$$\Delta\varepsilon < 10^{-5}$$

As the exchange-correlation potential was chosen approximation Kohn-Sham. For modeling framework was used nanowire ideal lattice of silicon, for example with transverse

dimensions 5x5 (sizes indicated in the unit cell parameters a=5.43A).

The distance between the quantum wires was commensurate with lateral dimensions of wires. The surface was passivated by hydrogen nanowire that helped to avoid the appearance of surface states in the bandgap.

Thus,the results of calculations electronic structure of quantum dimensional periodic matrix of silicon nanowires from first principles shows that the complete passivation of dangling bonds with hydrogen atoms leads to changes in band gap and properties of porous silicon.