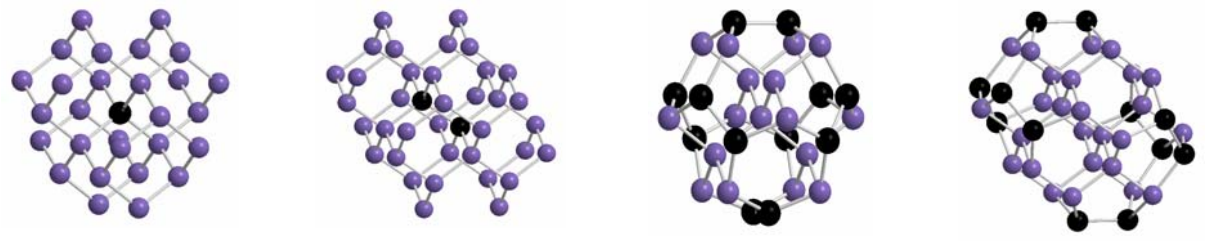
# QUANTUM CHEMICAL SIMULATION OF SURFACE EFFECTS IN NANOSILICON

**Normurodov A.B., Mukhtarov A.P., Sulaymonov N.T., Umarova F.T., Tereshchuk P.L**
*Institute of Nuclear Physics, Tashkent, Uzbekistan*

Silicon-based nanomaterials are predicted to have a great future in many areas, such as electronics, medicine and energy. The surface structure of silicon nanoclusters have a great influence on the electrical and optical properties of nanoparticles changing them drastically. Therefore, modeling of the surface structure of nanoparticles and their effects on various properties and microscopic electronic structure has a big importance.

In this paper we have presented the results of research of various surface structures of small silicon nanoparticles with diamond-like configuration by computer simulation of non-conventional tight-binding method [1]. Relaxation of atoms in the clusters is considered by stimulated annealing approach in the frame of molecular mechanics.

We consider two prototype diamond clusters: Si29, having in the center of an atom, and Si38, having in the center of Si-Si band. In Fig. also shows the diamond-like clusters with the dimerized surface structure (Si29D, Si38D).




The calculation results show that in the pure cluster the trimerization of the surface atoms are the most profitable. Trimerization as the dangling bonds of the surface atoms passivated becomes energetically unfavorable and the atoms undergo dimerization, which essentially consists in the formation of bonds between near neighbors of the surface. Dimerized and trimerized clusters have an elongated form, and their internal structure is disordered, rather close to the structure of amorphous silicon. Dimerized orbitals introduce an impurity band into the band gap of the cluster.

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1. Z. M. Khakimov. //Comput. Mater. Sci. 1994. V.3. P. 95-108.