Ab Initio Investigations of High-Pressure Behaviour of $Li_6B_4O_9$ Nanoclusters

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Numerous works on different physical properties of lithium tetraborate ($Li_2B_4O_7$) crystals point to promising possibilities for applications of these materials in acoustoelectronic devices, ultra-violet solid state lasers, and dosimetry. At the same time, atomic clusters can be building blocks of new nanostructured materials and, consequently, are of interest for intensive investigations with the prospect for applications in future nanotechnologies. At the same time, a study on the nanoparticles under high pressure is considered as a possible path to expand the range of available solid state materials. In this work, we present an *ab initio* theoretical analysis of the compression behaviour of lithium tetraborate nanoclusters.

The equilibrium geometries and energetic characteristics of free $Li_6B_4O_9$ cluster and of model ones where the $Li_6B_4O_9$ clusters are squeezed inside the spherical argon cages Ar_{30} have been calculated from the first principles. All the calculations were performed by means of the GAMESS (US) quantum chemistry package. The calculations on the total energy and equilibrium geometric structure were performed by the spin-restricted Hartree–Fock method (RHF) with the 6-31G valence-split basis set.

Our study is focused on the analysis of changes in the structure and properties of the confined $Li_6B_4O_9$ clusters upon their transition from the free state to the extremely compressed one. The hydrostatic pressure was simulated by reducing the diameter of the spherical argon cages in the range of 15 to 8 Å. *Ab initio* calculations with partial geometry optimization have been performed at each step of compression with a "frozen" cage Ar_{30}. According to the results of calculations, all the structures obtained of $Li_6B_4O_9@Ar_{30}$ clusters are stable and correspond to local minima of the potential energy surface. Under hydrostatic pressure which corresponds to the volume reduction (about $0.6V_0$) of $Li_6B_4O_9$ nanocluster, a transformation of cluster structure is observed.

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