$BaTiO_3$ based Nanostructures: Nanolayers, Nanotubes, Nanowires

Robert Evarestov

Department of Chemistry, Quantum Chemistry Division, St. Petersburg State University, Russia

e-mail: re1973@re1973.spb.edu

The first-principles LCAO calculations with hybrid HF-KS exchange correlation functional and the structure optimization are performed on the cubic $BaTiO_3$ based nanostructures: diperiodic (2D) layers with the periodicity in (001) and (110) planes, monoperiodic (1D) nanotubes (with the square morphology), monoperiodic (1D) nanowires with the translation axis along [001] and [110] directions. The convergence of the results with the nanosystem size increasing is studied under stoichiometric condition.

2D layers. $BaTiO_3$ (001) slabs, being consisted of even number of atomic planes with BaO and TiO_2 terminations, obey stoichiometry. Oxygen-terminated (110) slabs with odd number of planes can be converted to stoichiometric sheets by removing extra oxygen atoms from surface planes. The converged results for the surface energy of 1.28 J/m^2, 1.22 J/m^2, and the values for the formation energy of 24 kJ/mol, 33 kJ/mol are obtained for the (001) and (110) slabs consisting of 10 formula units.

1D nanotubes. The comparison of the surface and formation energies for the nanotubes rolled up from two (2L) and four (4L) planes (both with Ti and Ba terminations for the outer nanotube shell) is made. The monoperiodic unit cell consisting of 300 atoms was used to model the nanotubes with chiralities (60,0), (30,30) and (30,0), (15,15), respectively. The smallest surface energy (1.1 J/m^2) and the smallest formation energy (130 kJ/mol) were found for both 2L Ba terminated and 4L Ti terminated (30,0) nanotubes, respectively. The strain energy is about of –10 kJ/mol in the first case and +10 kJ/mol in the second case. The strain and formation energies of 4L nanotubes at chirality (n,n) are noticeably greater than those at chirality (n,0) for the both terminations.

1D nanowires. [001] nanowires were constructed using $n \times n \times 1$ supercells of the bulk crystal and removing the periodical boundary conditions in the [100] and [110] directions. For $n = 4$ (80 atoms in 1D unit cell) the surface and formation energies of [100] nanowire are 1.52 J/m^2 and 122 kJ/mol**,** respectfully. The results obtained for [110] nanowires are close to those for [001] nanowires of the equivalent size, except that their formation energy is slightly larger.

Author thanks St. Petersburg State University for the support (grant 12.37.142.2011).