Ab INITIO ENERGETICS OF LANTHANUM SUBSTITUTION IN FERROELECTRIC BISMUTH TITANATE

S. H. Shah
Theoretical Plasma Physics Division, Directorate of Science, PINSTECH, Nilore, Islamabad

Density functional theory based electronic structure calculations play a vital role in understanding, controlling and optimizing physical properties of materials at microscopic level. In present study system of interest is bismuth titanate ($Bi_4Ti_3O_{12}$)/(BIT) which has wide range of applications such as a high temperture piezoelectric and one of the best material for memory devices. However, it also suffers from serious issues such as oxygen vacancies which degrade its performace as a memory elelment and piezoelectric material. In this context, the bulk and defect properties of orthorhombic bismuth titanate ($Bi_4Ti_3O_{12}$) and bismuth lanthanum titanate ($Bi_{3.25}La_{0.75}Ti_3O_{12}$)/(BLT, x=0.75) were investigated by using first principles calculations and atomistic thermodynamics [1]. Heats of formation, valid chemical conditions for synthesis, lanthanum substitution energies and oxygen and bismuth vacancy formation energies were computed. The study improves understanding of how native point defects and substitutional impurities influence the ferroelectric properties of these layered perovskite materials. It was found that lanthanum incorporation could occur on either of the two distinct bismuth sites in the structure (Fig. 1) and that the effect of substitution is to increase the formation energy of nearby native oxygen vacancies. The results provide direct atomistic evidence over a range of chemical conditions for the suggestion that lanthanum incorporation reduces the oxygen vacancy concentration. Oxygen vacancies contribute to ferroelectric fatigue by interacting strongly with domain walls and therefore a decrease in their concentration is beneficial.

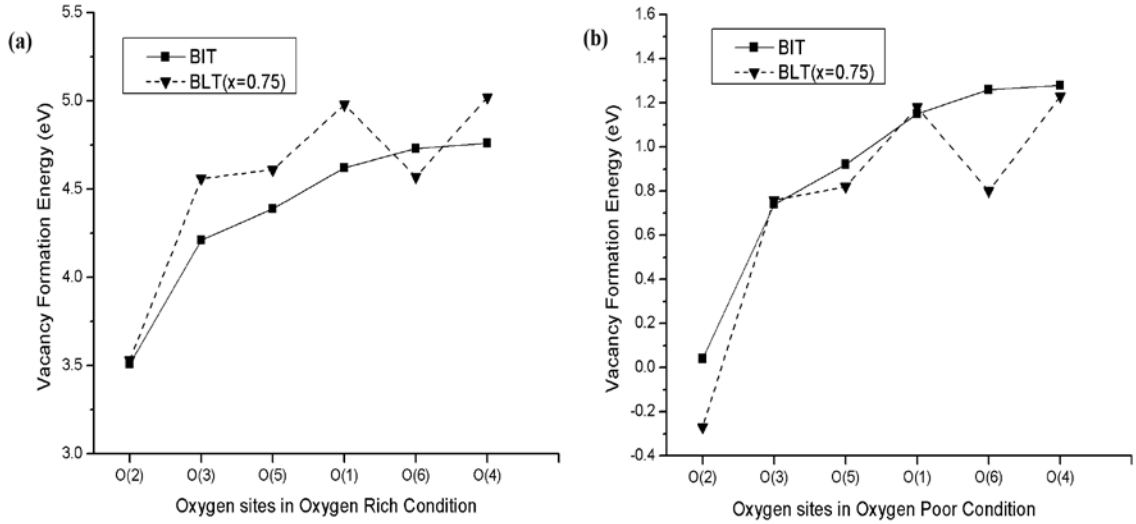

Fig. 1 Calculated oxygen vacancy formation energies at the six distinct sites O(1) to O(6) in BIT and BLT (x=0.75) under (a) oxygen rich and (b) oxygen poor conditions

Reference

1. S. H. Shah and P. D. Bristowe, "Ab initio energetics of lanthanum substitution in ferroelectric bismuth titanate", J. Phys. Condens. Matter **23** (2011) 155902.