SAIP 2011

Contribution ID : 144

Computational study of hematite(Fe_2O_3) and ilmenite($FeTiO_3$) structures

Wednesday 13 Jul 2011 at 17:00 (02h00')

Content :

We investigate the transformation from hematite to ilmenite structure by solid solution approach using ab initio quantum-mechanical simulation technique. The method uses the Density functional theory with the plane-wave (PW) pseudopotential method within the CASTEP code. We performed full structural relaxation allowing lattice parameters and cell violume to change to their mechanical equilibrium. We found that the transformation process does not change the structure (space group) as observed during geometry optimization. Our calculated properties i.e bond length, cell volume, lattice parameters, bulk modulus and density of states shows that hematite and ilmenite structures have similar property behavior with the lattice parameters corresponding to the experimental value, being large by 0.12%. The bond length from 20% to 50% shows the dominant of the Ti-O bond, in agreement with the experimental value. This bond length behavior is consistent with the density of state. However, we observe that the states overlap from VB to CB in VCA which is not expected from the experimental observations of the hematite and ilmenite crystal structures. The transformation from hematite to ilmenite structure due to doping was observed from 20% atomic titanium.

Level (Hons, MSc, PhD, other)? :

MSc

Consider for a student award (Yes / No)? :

Yes

Short Paper :

No

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