Contribution ID: **144** Type: **Poster Presentation**

Computational study of hematite(Fe₂O₃) and ilmenite(FeTiO₃) structures

Wednesday, 13 July 2011 17:00 (2 hours)

<p>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

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

No

Primary author: Mr MKHONTO, peace prince (University of Limpopo)

Co-authors: Dr ACKARMANN, Lutz (University of Limpopo); Prof. NGOEPE, phuti (University of Limpopo)

Presenter: Mr MKHONTO, peace prince (University of Limpopo)

Session Classification: Poster1

Track Classification: Track A - Condensed Matter Physics and Material Science