



Contribution ID: 265

Type: Poster

The Stability of High Pressure Phase of B₂O₃

The stability of boron trioxide is studied using the plane wave's pseudopotentials calculations. The hydrostatic pressure against volume at room temperature is being varied to determine the minimum energy possible for phase transformation. Our results agree well with various boron trioxide calculations and experiments.

Primary authors: Mr MOLOANTOA, Jacob (University of Limpopo); Dr MOSUANG, Thuto (University of Limpopo)

Co-author: Dr RAMMUTLA, Erasmus (University of Limpopo)

Presenters: Mr MOLOANTOA, Jacob (University of Limpopo); Dr MOSUANG, Thuto (University of Limpopo)

Track Classification: Track G - Theoretical and Computational Physics