Contribution ID: **241** Type: **Poster Presentation**

A Theoretical Investigation of the Structural, Electronic and Phase transition of Molybdenum Selenide compounds

Tuesday, 9 July 2013 17:40 (1 hour)

Abstract content
   (Max 300 words)

Molybdenum selenide structures may be potential may be potential materials for constructing solar cells. In this study, we numerically investigate the structural, electronic structure and pressure phase transition properties of some molybdenum selenide structures using density functional theory (DFT). Three DFT approximations are used to determine trends and properties. Pressure phase transitions up to 10 Gpa and elastic properties are examined to identify structurally stable systems. The electronic structure of the most stable systems are explored to determine the best potential candidates for solar energy harvesting.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

Professor Daniel P. Joubert, University of the Witwatersrand, Johannesburg. email: daniel.joubert2@wits.ac.za

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

No

Primary author: Mr ABDULSALAM, Mahmud (University of the Witwatersrand, Johannesburg)

Co-author: Prof. JOUBERT, Daniel (University of the Witwatersrand)

Presenter: Mr ABDULSALAM, Mahmud (University of the Witwatersrand, Johannesburg)

Session Classification: Poster1

Track Classification: Track A - Division for Condensed Matter Physics and Materials