



Contribution ID: 154

Type: Oral Presentation

First principles LDA + U and GGA + U study of protactinium and protactinium oxides: Dependence on the effective U parameter

Tuesday, 10 July 2012 15:10 (20 minutes)

Abstract content
 (Max 300 words)

The electronic structure and properties of Protactinium and its oxides (PaO and PaO₂) have been studied in the framework of the LDA, GGA(PBE), LDA+U and GGA(PBE)+U implementations of density functional theory. The dependence of selected observables of these materials on the effective U parameter has been investigated in detail. The examined properties include lattice constants, bulk modulus, effect of charge density distribution, hybridisation of the 5f orbital and energy of formation for PaO and PaO₂. The LDA+U gives a better agreement with experiment than the GGA+U for the structural properties of Pa. We obtained that PaO is metallic and PaO₂ is a Mott-Hubbard insulator within the DFT+U approximation. This is consistent with observations for other actinide oxides, unlike GGA and LDA which give metallic behaviour for PaO₂. The calculated band gap reported for PaO₂ is a prediction and should stimulate further studies.

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

Prof. Nithaya Chetty and nithaya.chetty@up.ac.za

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

No

Primary author: Mr OBODO, Kingsley (University of Pretoria, South Africa)

Co-authors: Prof. PRETORIUS, Jannie (University of Pretoria, South Africa); Prof. CHETTY, Nithaya (University of Pretoria, South Africa)

Presenter: Mr OBODO, Kingsley (University of Pretoria, South Africa)

Session Classification: DCMPM2

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