



Contribution ID: 483

Type: Oral Presentation

DFT+U study of Li adsorption on (110) β -MnO₂ surface

Friday, 12 July 2013 09:20 (20 minutes)

Abstract content
 (Max 300 words)

Lithium-air batteries are actively being developed worldwide because of their potential to deliver ultra-high energy density. Currently, the li-ion batteries are being used in electric vehicle however; their energy is much lower than that of Li-air batteries. Density Functional Theory is used to investigate lithium adsorbed manganese dioxide surfaces in the context of lithium-air battery development. In this study, we calculate the surface energies of low Miller index planes and the most stable surface orientation was found to be the (110). It was observed that the triply-coordinated lithium, bonded to two bridging and one in-plane oxygen atoms (bbp) has lowest adsorption energy which is the favorable site. Surface oxidation becomes favorable when concentration of lithium adsorbets increases at the surface of which bridging-peroxo is most stable.

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

No

Level for award
 (Hons, MSc,
 PhD)?

MSc

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

(P. E Ngoepe phuti.ngoepe@ul.ac.za)
University of Limpopo

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

No

Primary author: Ms MAENETJA, khomotso (University Of Limpopo)

Co-authors: Prof. NGOEPE, Phuti (University of Limpopo); Dr GRAU-CRESPO, Ricardo (University College London); Mr MELLAN, Thomas (University College London)

Presenter: Ms MAENETJA, khomotso (University Of Limpopo)

Session Classification: DCMPM1

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