Contribution ID: **248** Type: **Oral Presentation**

Advanced Power Sources for Electronic Devices and Electric Vehicles.

Wednesday, 10 July 2013 09:00 (20 minutes)

Abstract content
   (Max 300 words)

The growing global energy demand of modern society is urging to find large-scale sources, which are more sustainable and environmentally friendly of the oil-based ones. The increase of CO< sub >2< /sub > emissions and also the limited availability of oil, call for the search for sources of clean energy. Electrochemical systems for energy production, conversion and storage, including super capacitors, fuel cells and batteries, may play a relevant role. In particular, rechargeable lithium batteries are expected to play a key role also in future energy storage, including both stationary and automotive applications.
Li-ion batteries have transformed portable electronic devices. However, even when fully developed, the highest energy storage that this batteries can deliver is too low to meet the demands of key markets.
Reaching beyond the horizon of Li-ion batteries is a formidable challenge; it requires the exploration of new chemistry, especially electrochemistry and new materials. Here we consider a study on: Li-air, Li-S and Zn-air batteries. All this batteries are potentially viable ultrahigh energy density chemical power sources, which could potentially offer higher specific energy being rechargeable.
In the current work we present a comparative study on stability, structural and electronic properties of the discharge products of sulphur and oxygen formed in Li-air, Li-S and Zn-air batteries using planewave pseudopotential methods. Lattice parameters for the suggested compounds were calculated and compare well with experimental results. The elastic constants of all the discharge products of sulphur and oxygen formed in Li-air, Li-S and Zn-air batteries accord reasonably with experimental results, and the corresponding stability conditions are satisfied. Furthermore, the lattice dynamics of the products were calculated. The phonon dispersions of Li< sub >2< /sub >O and Li< sub >2< /sub >S suggested that the structures are stable and compare well with those obtained from neutron scattering experiments.

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

Yes

Level for award
 (Hons, MSc,
   PhD)?

MSc

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

Prof. P.E. Ngoepe
phuti.ngoepe@ul.ac.za
University of Limpopo-Material Modelling Centre

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

Yes

Primary author: Mr MASEDI, Cliffton (University of Limpopo-Material Modelling Centre)

Co-authors: Dr SITHOLE, Happy (CSIR); Prof. NGOEPE, Phuti (University of Limpopo-Material Modelling Centre)

Presenter: Mr MASEDI, Cliffton (University of Limpopo-Material Modelling Centre)

Session Classification: DCMPM1

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