Contribution ID: **90** Type: **Oral Presentation**

Computational modelling of graphene mediated sodium air batteries

Tuesday, 26 June 2018 12:00 (20 minutes)

Rechargeable metal–air batteries are widely regarded as the next best generation of high energy density electrochemical storage devices. The performance and rechargeability of these metal–air batteries is highly dependent on the stability and performance of the positive electrode materials, where oxygen reduction and evolution reactions occur. Due to the high cost and limited resources for lithium-ion batteries, sodium air batteries are a promising alternative because of their high theoretical energy density and low cost to meet the rapidly increasing global energy demands. Graphene has shown a great potential in electrochemical energy storage and conversion due to its remarkable properties. In this work, density functional theory (DFT) methodologies are used to investigate the reaction mechanisms of sodium oxides being adsorbed onto graphene surface. Generalized gradient approximation (GGA) as implemented in density functional theory was used to perform the calculations, employing CASTEP code. The four discharge products namely; Na₂O₂, NaO₂, Na₂O and NaO were adsorbed onto graphene layer. Our results show that Na₂O is the most stable discharge product due to its lower adsorption energy.

Please confirm that you
have carefully read the
abstract submission instructions
under the menu item
”Call for Abstracts”
(Yes / No)

Yes

Consideration for
student awards
Choose one option
from those below.
N/A
Hons
MSc
PhD

Hons

Supervisor details
If not a student, type N/A.
Student abstract submision
requires supervisor permission:
please give their name,
 institution and email address.

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

Primary author: Ms MORUKULADI, Mogahabo (UL)

Co-authors: Mr MASOGA, Phala (UL); Prof. NGOEPE, Phuti (UL); Prof. MAPHANGA, Regina (Csir)

Presenter: Ms MORUKULADI, Mogahabo (UL)

Session Classification: Physics of Condensed Matter and Materials

Track Classification: Track A - Physics of Condensed Matter and Materials