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Advanced Power Sources for Electronic Devices and Electric Vehicles.

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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 CO₂ 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 Li₂O and Li₂S suggested that the structures are stable and compare well with those obtained from neutron scattering experiments.

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

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

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

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

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