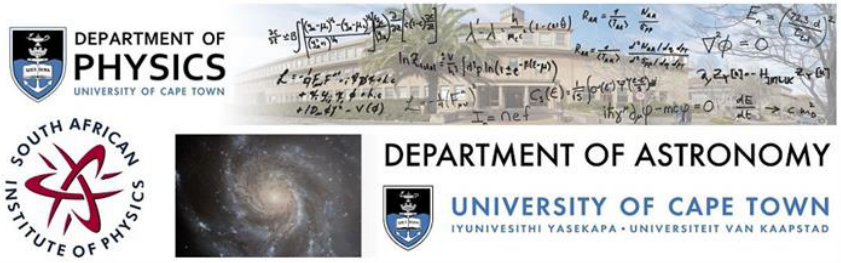

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Beyond Lithium-Ion Batteries: A Computational Study on Advanced Lithium – Sulphur Battery

Tuesday, 5 July 2016 10:20 (20 minutes)

Abstract content
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Rechargeable lithium–sulphur (Li–S) batteries hold great potential for high-performance energy storage systems because they have a high theoretical specific energy, low cost, and are eco-friendly.
We show the stability of Li₂S formed in Lithium- Sulphur batteries and investigate structural, electronic and mechanical properties using density functional theory within the generalized gradient approximation. Atomistic simulations was employed to successfully generate interatomic potential models. The lattice parameters were well reproduced and agree with the available experimental data. The heats of formation predicts that the structure Li₂S is generally stable. The elastic constants suggest that the structure is mechanically stable which is in great agreement with calculated phonon dispersion curve. Phonon dispersion curve shows that the structure is stable with absence of vibrations in the negative frequency and it is in good agreement with experiment work (neutron scattering experiments) and elastics properties which are all positive. The Buckingham interatomic potentials describing the interactions between lithium and sulphur were successfully generated and validated since they produced same melting temperature as experimental studies.

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Prof. Phuti Ngoepe
phuti.ngoepe@ul.ac.za
University of Limpopo
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Primary author: Mr MASEDI, CLIFFTON (CSIR/ UL)

Co-authors: Dr SITHOLE, HAPPY (CSIR/CHPC); Prof. NGOEPE, PHUTI (UL)

Presenter: Mr MASEDI, CLIFFTON (CSIR/ UL)

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