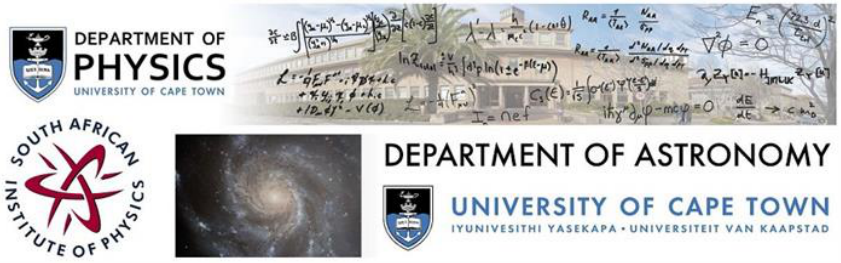

Contribution ID: **240** Type: **Oral Presentation**

Atomistic simulations studies on the structural change in Li_xTiO₂ (x: 2.82, 3.76, 6, 57) at high temperatures for energy storage in Lithium-ion Battery Applications.

Tuesday, 5 July 2016 14:00 (20 minutes)

Abstract content
   (Max 300 words)
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Molecular dynamics based amorphisation and recrystallisation technique was employed to produce lithiated nanosheet and porous structures of TiO₂ and to study their behaviour at high temperatures. Radial distribution functions and configuration energy vs time graphs, indeed showed that the structures architectures were highly twinned and reflected straight and zigzag tunnels corresponding to rutile and brookite polymorphs respectively. X-ray diffraction patterns of the nanosheet and nanoporous Li_xTiO₂ after recrystallization, also confirm the presence of rutile and brookite polymorphs. Lithium diffusion plots show that lithium ions diffuse well at elevated temperatures. Nanosheet and nanoporous pathways are able to accommodate more lithium ions and withstand high temperatures, hence affirming that such nanoarchitectures can be a good candidate for anodes of Li-Ion batteries.

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