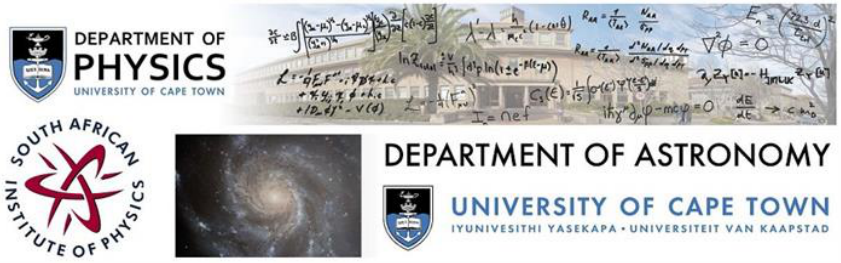

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Molecular dynamics studies of Lithium intercalation into amorphous structure of Titanium dioxide (TiO₂) nanoparticle

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
   (Max 300 words)
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Titanium dioxide (TiO₂) has been confirmed as a safe anode material in lithium ion batteries due to its higher Li-insertion potential, (1.5V) in comparison with commercialised carbon anode materials. Besides being used as an anode material it has a wide range of applications such as photo-catalysis, insulators in metal oxide, dye sensitized solar cells etc. In this work amorphous nanoparticle (NP) of TiO₂ comprising of 15972 atoms was lithiated with a different concentration of Lithium atoms. Simulation of amorphisation and re-crystallisation was employed to attain Li-TiO₂ nanoparticles and its microstructures. Molecular dynamics has been performed to crystallise all intercalated nanoparticles using the computer code DL_Poly. The crystallisation of the materials, starting from amorphous precursors, and the complex microstructure of the material was captured within each structural model including: polymorphic rutile and brookite structures, dislocations, grain boundaries, micro-twinning, vacancies, interstitials, surfaces and morphology. Microstructure depict the Lithium atoms situated on the tunnels and vacancies, shows that the material can store and transport Lithium during charging and discharging, making it an attractive anode material. Calculated X-Ray diffractions are in accord with the experimental data revealing the presence of brookite and rutile phases.

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