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Atomistic simulations studies on the structural change in Li_xTiO_2 (x : 2.82, 3.76, 6, 57) at high temperatures for energy storage in Lithium-ion Battery Applications.

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Abstract content
 (Max 300 words)
Formatting
Special chars

Molecular dynamics based amorphisation and recrystallisation technique was employed to produce lithiated nanosheet and porous structures of TiO_2 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_xTiO_2 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 nano-architectures can be a good candidate for anodes of Li-Ion batteries.

Apply to be considered for a student award (Yes / No)?

yes

Level for award (Hons, MSc, PhD, N/A)?

Msc

Main supervisor (name and email) and his / her institution

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