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Atomistic simulation studies of Lithium intercalation into amorphous structure of TiO₂ nanoporous

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Due to its wide band gap Titanium dioxide (TiO₂) has variety of applications such as photo-catalysis, dye sensitized, energy storage, etc. In this work amorphous nanoporous structure of TiO₂ consisting of 15 972 atoms has been generated and lithiated with different concentration of Lithium atoms for Lithium ion batteries (LIB). Amorphisation and re-crystallisation technique was employed to attain Li-TiO₂ nanoporous and its microstructures. Molecular dynamics simulation has been performed to crystallise all intercalated nanoporous using the computer code DL_Poly. Lithiated nanoporous structures was annealed to 0 K. Microstructures reveal Li atoms on the surface entrance sites and on channel of the structure, which makes the material a good anode material for LIB. It also indicate that nanoporous can store and transport Li atoms during charging and discharging. X-ray diffractions indicate that our system has brookite and rutile phases which accord well with the experimental data.

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

no

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

n/a

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

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Would you like to submit a short paper for the Conference Proceedings (Yes / No)?

yes

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