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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.

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

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yes

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