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Structural evolution and ion diffusion of TiO₂ nanosheet at different temperatures for anode material Li-ion batteries.

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The structural evolution of TiO₂ nano-sheet is investigated by molecular dynamics code upon heating up to crystallization. The structural rearrangements during cooling and heating process are analysed as a function of temperature, focusing on shift of the peaks in X-ray diffraction and radial distribution function. Diffusion Coefficients of Li are measured to be increasing with an increase in temperature. The structure of TiO₂ nano-sheet was maintained at elevated temperatures as observed on their micro-structure and XRD's. Thus rendering suitable anode material for Li – ion batteries since it can withstand such temperatures.

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

yes

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