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Computational modelling studies of recrystallised nano-architectured TiO2 structures at different lithium concentration and temperatures for energy storage applications.

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Abstract content
   (Max 300 words)
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TiO₂ is a safe anode material in lithium ion batteries due to its higher Li-insertion potential of 1.5V when compared with the commercialised carbon anode materials [1]. In this study we investigate how the structure of the lithiated nano-architecture structure of titanium dioxide behaves at different lithium concentration as the structure recrystallises. It is observed that lithiation tends to armophised the structure in accordance with pair distribution function experiments. X-ray Diffraction pattern was produced and compared with the experimental XRD's.Microstructure was generated and found to be highly twinned hence forming straight and zigzag tunnels.

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yes

Level for award
 (Hons, MSc,
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Msc

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

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