Abstract Submitted
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Atomistic Simulation Studies of the Bulk Lithiated TiO_2[1] PHUTI NGOEPE, MALILI MATSHABA, University of Limpopo, DEAN SAYLE, University of Cranfield — TiO_2 has been confirmed as a safe anode material in lithium ion batteries due to its higher Li-insertion potential, (1.5V) in comparison with commercialised carbon anode materials. In the current study, amorphisation recrystallization method is used to produce bulk TiO_2 with a brookite structure and lithium is inserted at different concentrations. In accordance with pair distribution function experiments [1], it is found that lithiation tends to amorphise the structures. Simulated X-ray diffraction patterns are produced from such structures and compared with the experimental XRDs. Microstructures of TiO_2 are generated and are found to be highly twinned hence forming straight and zigzag tunnels. The microstructures of lithiated TiO_2 display limited twinning and tunnels with less pathways available for lithium transport. The microstructures are compared with those of nanostructural TiO_2 and suggestions for the preference of the latter in anodes are put forward.

[1] D. Dambournet, K. W. Chapman, M.V. Koudriachova, P.J. Chupas, I. Belharouak, and K. Amine, Inorg. Chem. 2011, 50, 5855–5857.

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