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Atomistic simulation studies of lithiated and sodiated TiO2 nanoarchitectures. PHUTI NGOEPE, KENNETH KGATWANE, MALILI MATSHABA, Unviersity of Limpopo, Sovenga, 0727, South Africa, DEAN SAYLE, University of Kent, Canterbury, CT2 7NZ, UK — Simulated amorphisation recrystallization methods, are now routinely used to generate models of various nanoarchitectures for metal oxides with complex microstructural details [1]. Herein, we present a detailed simulated synthesis for nano-architectures of mixed TiO_2 brookite and ruitle polymorphs as anode material for Li-ion, and Na-ion batteries. Volume changes associated with electrochemical insertion during charging are predicted. The resulting nanostructures are characterised from visual images, radial distribution functions, XRDs and simulated microstructures. Discussions on amounts of Li- and Na-ions that can be accommodated in such nano-architectures and how they influence ion transport are presented. [1] M.G. Matshaba, D.C. Sayle, T.X.T. Sayle and P.E. Ngoepe, J. Phys. Chem. C, (2016), 120, 14001.

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