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SIMULATIONS SYNTHESIS OF Na0.23TiO2 NANOSPHERE AT VARIED TEMPERATURES: BEYOND LI-ION BATTERIES.

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Sodium-ion batteries (NaIBs) have been widely used in energy storage applications such as portable devices and electric vehicles [1]. The demand of lithium rapidly increases year by year, pushing up the price and making lithium resources less affordable. Thus, it is crucial to find alternative technology beyond Li-ion batteries (LIBs) employing abundant elements on earth. Sodium (Na+) becomes a suitable candidate due to its high abundance and low cost as well as the similar redox potential to lithium [1]. Generated TiO2 nanosphere-architectured [2] are promising as anode electrode materials for Na+ rechargeable batteries due to their capacity to host more Na+ ions and withstand high temperature conditions. In these study, simulation recrystallisation of nanosphere Na0.23TiO2 structure was synthesised from an amorphous precursor by running large scale molecular dynamics (MD) method using DL_POLY_2 code [3] to predict their structural stability at varied temperatures. Recrystallisation synthesis, was then proceeded by the cooling process towards 0 K, the cooled Na0.23TiO2 nanosphere structure was then heated from 100 K to 2000 K at temperature intervals of 100 K using an NVT Nose Hoover ensemble. The calculated Ti - O pair correlation was evaluated by their Radial Distribution Functions (RDF's), where the extent of crystallisation was confirmed during cooling synthesis. The simulated X-ray diffraction (XRDs) spectra agreed well with the experimental XRD's of pure TiO2 [4], as well with the modelled microstructural defects, which all exhibited peak domains patterns of both rutile and brookite polymorphic phases, thus enhancing structural stability and energy storage characteristics. The Na+ ions transport showed an increase with an increase in temperature and maximum diffusion coefficients and activation energies of 110 x10-9 m2s-1 and 0.190 eV respectively was calculated to track the rate of Na+ ion transport in the nanosphere TiO2 structures. These results provide substantial new improvements and insights that Na0.23TiO2 nanosphere structures is an excellent anode electrode candidate for sodium ions batteries (NaIBs), since it stored more Na+ ions and have withstands high temperatures conditions without compromising their internal microstructures.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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