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Atomistic simulation studies of NaxTiO2 nanoporous-architecture for future anode electrode materials in sodium ion batteries.

Recently, the attention to sodium-ion batteries has been refocused on large-scale energy storage applications, due to sodium's low cost and infinite abundance. The current study focuses on the effects of high temperatures on nanoporous Na -TiO2 within the temperature ranges of 0 K -2000K. Molecular dynamics simulations studies were carried out using the DL_POLY 2.20 code on South Africa's Centre for High Performance Computing Lengau supercomputers with 192 CPU on OpenMPI. Simulated amorphisation and recrystallisation technique was used to derive microstructural and radial distribution functions models for nanoporous Na0.03TiO2, Na0.04TiO2, Na0.07TiO2 comprising of 16122, 16172 and 16322 atoms respectively. Recrystallisation took longer period than expected on all three systems which then became our major challenge. Each models were cooled from 1500 K to 0 K within 500 K interval. The resulting models conformed to the rutile and brookite polymorphs which are good properties for storing energy as an anode electrode sodium ion batteries.

Presenter Biography

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