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ATOMISTIC SIMULATION STUDY OF SODIUM INTERCALATION IN TITANIUM DIOXIDE NANOSTRUCTURES

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Sodium-ion batteries (NIBs) have emerged as a promising candidate for application in large scale energy devices. These batteries have the same battery configuration as lithium–ion batteries (LIBs), however the huge difference in the ionic size, makes it impossible for graphite (anode material in LIBs) to intercalate sodium ions. Therefore it is crucial to develop high-performance anode materials for NIBs. We investigate the potential of titanium dioxide (TiO₂) nanosphere as an anode material for NIBs since TiO₂ is highly stable with most organic electrolytes, has small structural changes during intercalation, it is nontoxic and inexpensive.TiO₂ nanosphere was sodiated with a total of 300 atoms and investigated the structure from amorphous to crystalline phase while varying temperature. Recrystallization was achieved by using molecular dynamics (MD) simulation with the DL_POLY code this was confirmed by the configurational energy plots. The structural rearrangement during cooling to 0K were analysed by radial distribution functions (RDFs) and the microstructures thereof shows the presence of sodium vacancies, rutile and brookite polymorphs, these polymorphs were also observed on the XRDs. Our study shows that sodium ions can be intercalated in Na_{0.06}TiO₂ nanosphere, thus TiO₂ nanosphere can serve as suitable anode material for sodium ion batteries.

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