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Atomistic simulation studies of LixTiO2, NaxTiO2 and MgxTiO2 (x=0.11,0.15,0.19 and 0.23) nanosphere for metal ion batteries: Beyond lithium-ion Batteries.

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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 lithium-ion batteries (LIBs) that employs abundant elements on earth. Sodium (Na+) and magnesium (Mg2+) are suitable candidates due to their high abundance and low cost, as well as their compatible redox potential to lithium [1]. Generated TiO2 nanosphere architectured [2] are very promising as anode electrode materials for rechargeable batteries due to their ability to host more single (Li+ and Na+) and divalent (Mg2+) ions under highly extreme temperature conditions. In these studies, the simulation recrystallization of the LixTiO2, NaxTiO2 and MgxTiO2 nanosphere with x = 0.11,0.15,0.19 and 0.23 was atomistically synthesized from an amorphous precursor through the large-scale classical molecular dynamics (MD) method using the DL_POLY code [3] to predict its structural stability at varied temperatures. Recrystallisation synthesis was then proceeded by the cooling process towards 0 K; the cooled LixTiO2, NaxTiO2 and MgxTiO2 nanosphere structures were then heated from 100 K to 2000 K at temperature intervals of 100 K using an NVT Nose Hoover ensemble (exothermic reaction). The calculated correlation of the Ti - O pair was evaluated by their Radial Distribution Functions (RDFs), where the extent of crystallization was confirmed mostly after cooling synthesis. The simulated X-ray diffraction (XRDs) spectra agreed well with the experimental XRD's of pure TiO2 polymorphs [4], as well with the modelled respective microstructural defects, which all exhibited peak domains patterns of brookite (zigzag tunnels), anatase (complex tunnels) and rutile (straight tunnels) at all varied temperatures and Li+, Na+ and Mg2+ concentrations which are good properties for enhancing structural phase stability and energy storage capabilities. The Li+ and Na+ diffusivity rates within the TiO2 nanosphere both indicated a rapid increase in diffusion coefficients, Li+ had the highest diffusion coefficients more than that of Na+ and Mg2+ at all varied temperature and varied ion concentration. However, the sudden drop in Li and Na diffusivity rates on Li0.19TiO2 and Na0.19TiO2 nanosphere structures was due to the highly amorphous atom connectivity formed after all simulation synthesis. Furthermore, Mg2+ had a constant zero diffusion coefficients at all increased temperatures and ion concentrations within the TiO2 nanosphere. These results provide substantial new improvements and insights that LixTiO2, NaxTiO2 and MgxTiO2 nanosphere structures are an excellent candidate as anode electrode materials for lithium ions batteries (LIBs), sodium ions batteries (NaIBs) and magnesium ions batteries (MgIBs), due to their capabilities of storing more Li, Na and Mg atoms and withstanding highly extreme temperatures conditions while maintaining their structural phase stability and atom ordering to improve the battery performance.

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

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