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Computer Simulation Studies of Spinel $LiMn_2O_4$ Nanotubes

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Abstract : Nanostructured materials are attractive candidates for efficient electrochemical energy storage devices because of their unique physicochemical properties. Nanotubes have drawn a continuous attention because of their unique electrical, optical and magnetic properties contrast to that of bulk system. They have potential application in the field of optical, electronics and energy storage device. Introducing nanotubes structures as electrode materials; represents one of the most attractive strategies that could dramatically enhance the battery performance. Spinel LiMn2O4 is the most promising cathode material for Li-ion batteries. In this work, computer simulation methods are used to generate and investigate properties of spinel LiMn2O4 nanotubes. Molecular dynamic simulation is used to probe the local structure of LiMn2O4 nanotubes and the effect of temperature on these systems. It is found that diameter, Miller indices and size have a direct control on nanotubes morphology. Furthermore, it is noted that stability depends on surface and wrapping of the nanotube. The nanotube structures are described using the radial distribution function and XRD patterns. There is a correlation between calculated XRD and experimentally reported results.

Keywords : LiMn2O4, li-ion batteries, nanotubes, nanostructures
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