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# Computer simulation study of spinel LiMn<sub>2</sub>O<sub>4</sub> nanotubes as a cathode material for lithium-ion batteries

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## Abstract content <br>   (Max 300 words)<br><a href="http://events.saip.org.za/getFile.py/a target="_blank">Formatting &<br>Special chars</a>

Improvement of the energy density and power density of the lithium-ion batteries is urgently required with the rapid development of electronic devices. Developing nanostructured electrode materials represented one of the most attractive strategies to dramatically enhance battery performance. Spinel LiMn<sub>2</sub>O<sub>4</sub> is one of the most important promising cathode materials due to its nontoxicity and its low cost. In these paper, computer simulation methods are used to generate various structures of spinel LiMn<sub>2</sub>O<sub>4</sub> nanotubes, where index, size, symmetry and diameter are varied. Molecular dynamics simulation is used to investigate the local structure of spinel LiMn<sub>2</sub>O<sub>4</sub> nanotubes and the effect of temperature on the generated systems. It was found that diameter, symmetry, size, orientation and miller index have a direct control on nanotube morphology and stability depends on surface and termination. The nanotube structures are described using the radial distribution functions and XRD patterns. The calculated XRD patterns are in agreement with experimental results.

## Apply to be<br> considered for a student <br>   award (Yes / No)?

yes

## Level for award<br> (Hons, MSc, <br>   PhD)?

MSc

## Main supervisor (name and email)<br>and his / her institution

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## Would you like to <br> submit a short paper <br> for the Conference <br> Proceedings (Yes / No)?

no

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