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Computer Simulation Study Of Manganese Dioxide Nanotubes

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Abstract content
   (Max 300 words)

The field of nanotubes is undergoing an explosive growth, fueled by a breakthrough in synthesis and promise of unique applications. Manganese dioxide is a widely used material in supercapacitor because of low-cost and high energy density. Manganese dioxide nanotubes play an important role in electrochemical applications, including serving as cathode material in lithium-ion batteries. Computer simulation methods were used to generate various structures of manganese dioxide nanotubes, where index, size, symmetry and diameter are varied. Molecular dynamics was used to investigate the local structure of manganese dioxide nanotubes at different temperatures ranging from 300K to 3300K. The nanotubes structures were described using the radial distribution function. The structural stability of nanotubes generated from low index surfaces was investigated and found that {110} surface produced the most stable nanotube.

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