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Computer simulation as a strategy for generating manganese dioxide nanotubes

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Abstract content
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Nanostructured materials are attractive candidates for efficient electrochemical energy storage devices because of their unique physicochemical properties. Introducing nanotube systems as electrode materials represents one of the most attractive strategies that could dramatically enhance the battery performance. Nanostructured manganese dioxide has been considered as an ideal electrode material for energy storage devices such as high-energy and power lithium-ion batteries. In this paper, computer simulation strategy is used to generate various structures of manganese dioxide nanotubes by varying Miller index and diameter and determine their effect on nanotube generation. It is found that diameter and Miller index have a direct control on nanotube morphology and stability of generated models depends on the surface and termination. Molecular dynamic simulation is further used to investigate the structure of manganese dioxide nanotube and the effect of temperature on the generated systems. Molecular graphical images showing the atomic positions for the nanotubes are presented and the nanotube structures are described using radial distribution functions and XRD patterns. The calculated XRD patterns are in good agreement with the experiments, thus validating the generated structural models for the nanotubes. The resulting models conforms to pyroluiste polymorph of manganese dioxide, featuring octahedrally coordinated manganese atoms.

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