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Computer simulation studies of SPINEL LiTi₂O₄

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Abstract content
   (Max 300 words)

The spinel LiTi₂O₄ system is of interest in battery applications and used as an anode material... Molecular dynamics calculations were carried out to investigate the effects of temperature on spinel lithium titanate. The NVE ensemble was used, whereas the temperature was varied, ranging from 300K-3000K. The radial distribution functions, diffusion coefficient and x-ray diffractions were analysed. It was observed that the LiTi₂O₄ system undergoes structural transformation from spinel to ramsdellite at 1148.15K, which gives a good agreement with experimental data acquired.

Apply to be
 considered for a student
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no

Level for award
 (Hons, MSc,
   PhD)?

Hons

Main supervisor (name and email)
and his / her institution

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Would you like to
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no

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