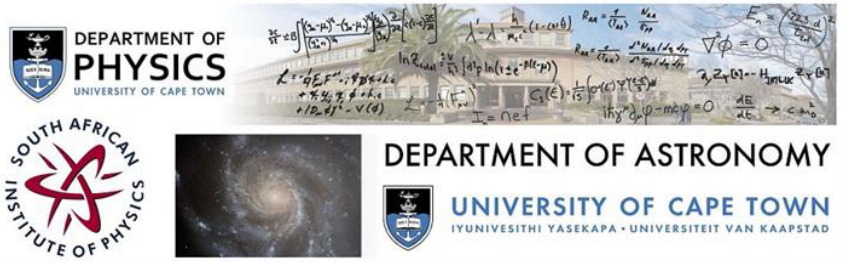

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Computer simulation studies of spinel LiMn₂O₄ surfaces

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Abstract content
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Lithium ion batteries are important electrochemical energy storage devices for consume electronics and the most promising candidate for electric and hybrid electric vehicles. The surface chemistry influences the performance of the batteries. Consequently, stable surface is a basic requirements for a perfect cathode material. The surface structures {100}, {110} and {111} of the spinel LiMn₂O₄ were investigated using computer simulation methods. In particular, density functional theory calculations within the generalised gradient approximation was used to determine surface structures and stability of LiMn₂O₄. The effect of surface termination and number of layers was determined. It was found that the surface termination and slab construction play a key role in determining the relative stability of {100}, {110} and {111} surfaces. Following the investigation of possible surface terminations and surface layer construction, results showed that {111} Li-termination surface is the most stable surface. The Wulff morphology of LiMn₂O₄ was constructed exhibits a cubo-octahedral shape with {111} facets dominating the morphology, in agreement with experimental studies.

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