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Atomistic Simulation Studies of Lithiated MnO2 Nanostructures

MnO2 has found extensive applications as a cathode material in lithium batteries. However MnO2 suffers from structural degradation during charge/discharge which leads to capacity fading. We use atomistic simulation to explore and mitigate this structural collapse by employing novel porous MnO2 nanostructures with defects. The nanostructures are lithiated to simulate charge/discharge.

Primary author: Mr KGATWANE, Kenneth (University of Limpopo)

Co-authors: Prof. SAYLE, Dean (Cranfield University); Prof. NGOEPE, Phuti (University of Limpopo); Dr MAPHANGA, Regina (University of Limpopo)

Presenter: Mr KGATWANE, Kenneth (University of Limpopo)

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