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Atomistic Simulation Study of Lithium Manganese Oxides for Li-Ion Batteries PHUTI NGOEPE, KENNETH KGATWANE, RAPELA MAPHANGA, Materials Modelling Centre, Private Bag x1106, University of Limpopo, Sovenga 0727, South Africa, THI SAYLE, DEAN SAYLE, DEAS, Cranfield University, Defence Academy of the United Kingdom, Shrivenham, Swindon, SN6 8LA, UK. — Simulated amorphisation recrystallisation (A+R) technique has been successfully used to generate models of various nano-forms of the complex manganese dioxides [1]. We apply the method to study lithium insertion into the nano - spheres, sheets, rods and porous structures of the binary MnO_2. The variation of mechanical properties and microstructural features with lithium concentration are investigated. The bulk ternary Li_2MnO_3 provides structural integrity for lithium-ion battery cathodes and is electrochemically inactive. The nanocrystalline Li_2MnO_3 has a structure similar to that of the bulk, but shows different lithium intercalation properties [2]. We simulated such a nanophase by the A+R method, and the resulting microstructures provide insights into the origins of the electrochemical activity which renders it suitable for battery electrodes.

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