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Atomistic Simulation of Lithiated Mesoporous Manganese Dioxide PHUTI E. NGOEPE, Materials Modelling Centre, Private Bag x1106, University of Limpopo, Sovenga 0727, South Africa, THI X. SAYLE, DEAN C. SAYLE, DSSR, Cranfield University, Defence Academy of the United Kingdom, Shrivenham, Swindon, SN6 8LA, UK — Recent studies have shown that mesoporous manganese dioxide is capable of reversibly storing specific capacity of 284 mAh/g. Atomistic simulated amorphisation recrystallisation technique, involving tens of thousands of atoms, has been successfully used to generate models of various nano-forms of the complex manganese dioxide, which include microstructural details. In the current study, we will apply the method to the study of lithiated mesoporous structures. We observe microstructural features that compare well with the high resolution electron microscopy mirographs. We also use the atomistic simulations to explore the mechanical strength of porous nanomaterials. We show that mesoporous manganese dioxide undergoes a significant volume expansion when Li is fully intercalated, which can only be sustained without structural collapse, if the nano-architecture is symmetrically porous, enabling elastic deformation during intercalation

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