Abstract Submitted
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**Atomistic simulation studies of nanostructured Li2MnO3** PHUTI NGOEPE, University of Limpopo, Sovenga, 0727, South Africa, THI SAYLE, DEAN SAYLE, University of Kent, Canterbury, CT2 7NZ, UK — The structures of the lithium-rich layered materials are basically derived from the layered rock-salt a- NaFeO2 type structure with space group R-3m. Nano-sized crystalline cathode material, Li2MnO3, was prepared by single step hydrothermal reaction [1]. The prepared materials delivered a high electrochemical reversible capacity charged/discharged between 2.0-4.3V, which indicates their promising future potential. In the current study simulated amorphisation recrystallisation method [2] is used to nucleate and crystallise ternary a nanoparticle of Li2MnO3, which is an end member compound of composites. The generated structure is characterized and the Li layer is found to accommodate some Mn ions. The latter is explained in terms of heats of formation deduced from DFT calculations. Microstructural features and transport properties are presented and a possible origin of the electrochemical activity is discussed. [1] G. R. Liu, S.C. Zhang, X. X. Lu, X. Wei, Proceedings Int. Conf. Nanomaterials: Applications and Properties, Vol. **2,** No 2, 02PCN25(3pp) (2013). [2] P.E.Ngoepe, R.R. Maphanga and D.C. Sayle, (2013), "Towards the Nanoscale", Chapter 9 in Computational Approaches to Energy Materials, pp 261-290, edited by C.R.A. Catlow, A. Sokol and A. Welsch, John Wiley and Sons Ltd.

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