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Comparison of electrochemical activity in nanoporous and bulk β-MnO_2 PHUTI NGOEPE, University of Limpopo, Sovenga, 0727, South Africa, THI SAYLE, University of KentCanterbury, CT2 7NZ, UK,, DEAN SAYLE, University of Kent, Canterbury, CT2 7NZ, UK — Simulated amorphisation recrystallisation method has been successfully used to nucleate and crystallise bulk [1] and nanoporous β-MnO_2 [2]. In the current study molecular dynamics simulation reveals that the reason nanoporous β-MnO_2 is electrochemically active, in contrast to the parent bulk material, is because strain imposed upon nanoporous β-MnO_2 during lithium intercalation does not influence the structure or dimensions of the 1D tunnels in which the lithium ions intercalate and reside. Conversely, the parent bulk material suffers structural collapse of the 1D tunnels under strain.

[1] T.X.T. Sayle, C.R.A. Catlow, R.R. Maphanga, P.E. Ngoepe and D.C. Sayle, *J. Crystal Growth*, **294**,118-129, 2006.
[2] T.X.T. Sayle, R.R. Maphanga, P.E. Ngoepe and D.C. Sayle, *J. American Chem. Soc.*, **131**, 6161-6173, 2009.

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