Atomistic Simulation Studies on Lithiation of MnO_2 Nano-architectures

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Nanostructured manganese dioxides (MnO_2) are among the promising materials for high-capacity lithium-ion batteries [1], lithium air batteries [2] and supercapacitors [3], that can be used in electric vehicles and other consumer electronics. They further have several advantages owing to their high specific energy capacity, low fabrication cost, abundance of the materials in the earth, and environmentally friendly nature [4]. Various experimental methods have been employed for the synthesis of MnO_2 with various nano-architectures such as the spheres, sheets, porous [5], wires, rods [6] etc.

Atomistic simulation methods provide a unique platform of exploring structural features at the nanoscale. Crystallised nano-architectures i.e. sphere, rod, sheet and porous MnO_2 consisting of 25000 atoms, and grown by simulated amorphisation crystallisaiton method [5], were lithiated by inserting 0 to 6000 Li ions. The volume change with Li content was investigated by performing molecular dynamics simulation under various ensembles. The variation of structural properties and related microstructural features with low and high lithium concentration are discussed. Associated changes provide valuable insights on the impact of charging and discharging in electrodes of such lithium ion batteries.

References

[1] B.X. Li, G.X. Rong, Y. Xie, L.F. Huang and C.Q. Feng, Inorg. Chem. 2006, **45**, 6404.
[2] A. Débart, A.J. Paterson, J. Bao and P.G. Bruce, Angew. Chem., Int. Ed. 2008, **47**, 4521.
[3] W. Wei, X. Cui, W. Chen and D.G. Ivey, Chem. Soc. Rev. 2011, **40**, 1697.
[4] S. Devaraj and N. Munichandraiah, J. Phys. Chem. C 2008, **112**, 4406.
[5] J.H. Cheng, G.A. Shao, H.J. Yu and J.J. Xu, J. Alloys Compd. 2010, **505**, 163.
[6] X. Wang and Y. Li, Chem. Eur. J. 2003, **9**, 300.
[7] 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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