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Strain-induced tuning of surface energetics, electron conductivity and reduction drive in spinel $LiMn_2O_4$ cathodes[1] IVAN SCIVETTI, GILBERTO TEOBALDI, University of Liverpool — $LiMn_2O_4$ (LMO) implementation in cathodes of rechargeable Li-ion batteries (LIBs) is hampered by the limited lifetime of the material and the stability of its interfaces, starting from the Solid Electrolyte Interphase [1,2]. Recent experiments [2] and Density Functional Theory (DFT) simulations [3] indicate that the formation and effectiveness of the SEI on LMO are related to the surface orientation. In this context, we analyse the role of geometrical strain for the relative energy, magnetic ordering and the reduction drive of several LMO surfaces. DFT simulations reveal LMO surfaces to be markedly sensitive to geometrical strain. Strain lower than 10% can lead to insulator-metal and ferromagnetic-antiferromagnetic transitions, alter the relative energy of LMO surfaces, and induce changes as large as 1.0 eV in the surface chemical potential, thence the reduction drive. Prompted by advances in the synthesis of metal-oxide core-shell nanostructures [4], the use of strained LMO coating to enhance SEI-formation is put forward as a potential nano-engineered strategy for longer lived SEI on LMO substrates.

1. JCPC 2012, 116, 9852-9861
2. J. Am. Chem. Soc. 2010, 132, 15268-15276
3. J. Phys. Chem. C 2015, 119, 21358-21368
4. ACS Nano 2012, 6, 5531.

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