Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Lithium diffusion study in Li_2MnO_3 and $Li_{1.17}Ni_{0.17}Mn_{0.67}O_2$: a combine experimental and computational approach†

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1 Experimental details

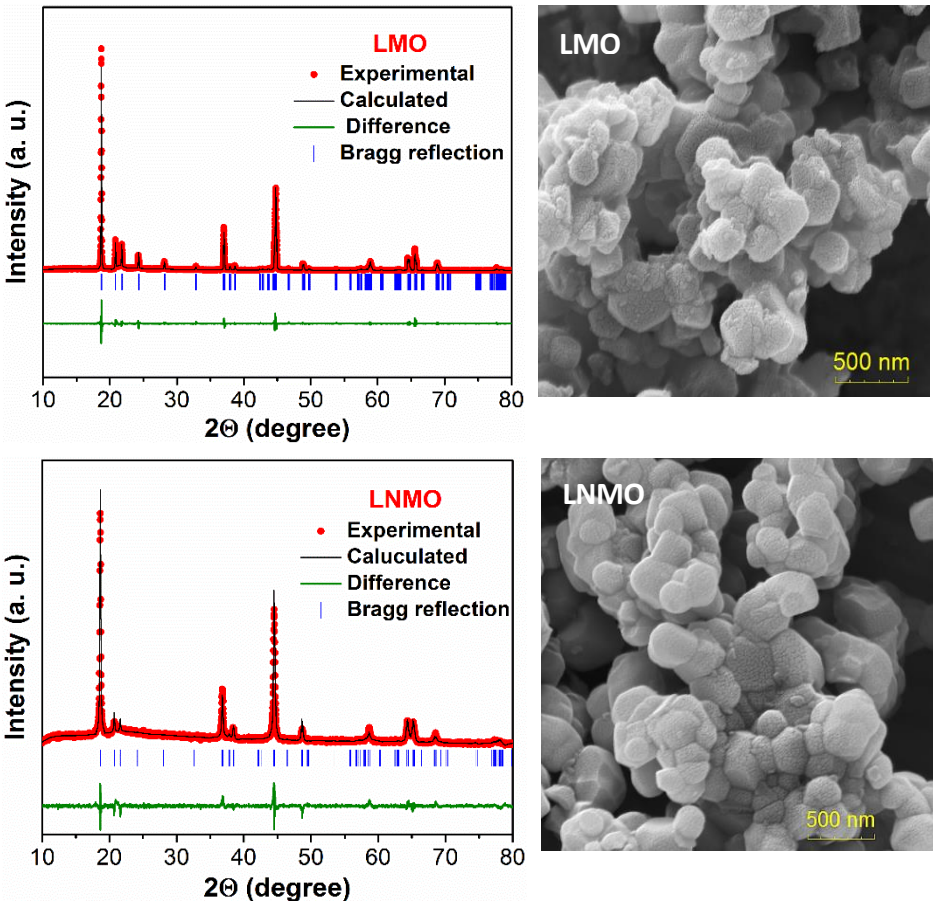

Fig. S1 Rietveld refinement fitting of X-ray diffraction pattern of both LMO and LNMO phases showing the experimental data points (red), calculated pattern (black), their difference (green), Bragg diffraction positions (blue tick marks) and SEM (scale bar is 500 nm) images of as prepared LMO and LNMO powder samples.

The powder XRD pattern of both LMO and LNMO and their Rietveld fit were shown in Fig. S1. All the reflections were indexed in a monoclinic cell with a space group C2/m. FESEM

images of both the powder samples shown in Fig. **S1** exhibit uniform morphology with agglomeration of the particles of size in the range 100–300 nm.

2 Theoretical details

2.1 Energy barrier profile

For $d_{2b\text{-}4h}$ diffusion path of Li_2MnO_3 (Fig. 1a from main manuscript), Li diffusion from Li4 position to Li14 position is considered to study the diffusion barrier. In the process to calculate diffusion barrier, four coordinates of Li have been created between Li4 and Li14. Each Li coordinate present in four different Li_2MnO_3 structures. Later, all the structures are optimized with nudged elastic band (NEB) method[1]. The relative value of total energy between one structure to another is calculated. These values are plotted with the distance between two Li atoms in the energy profile. Similarly, all the energy profiles have been generated for both the compounds.

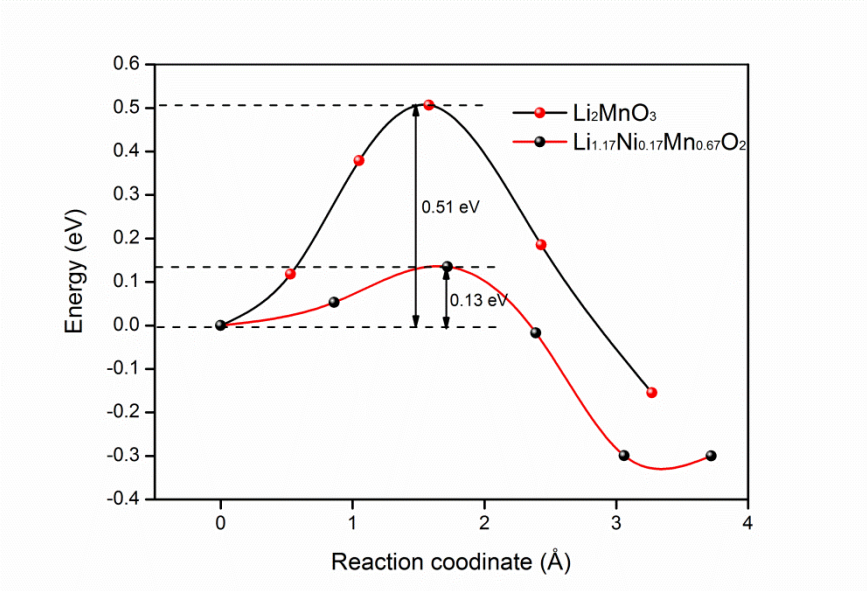

Fig. S2 Energy barrier profile on single Li diffusion along $d_{2b\text{-}2c}$ in LMO and LNMO.

Table S1 Bond sum value of Li in Li_2MnO_3 and $Li_{1.17}Ni_{0.17}Mn_{0.67}O_2$

	Bond sum value	
	Li_2MnO_3	$Li_{1.17}Ni_{0.17}Mn_{0.67}O_2$
Li in 2c site	1.03	1.08
Li in 2b site	1.11	1.00
Li in 4h site	1.02	0.94

References

1 H. Jonsson, G. Mills and K. W. Jacobsen, *Classical and Quantum Dynamics in Condensed Phase Simulations*, edited by D. Chandler, B. J. Berne, G. Ciccotti, and D. F. Coker (World Scientific, Singapore, 1998), 385–404.