Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

New allotropes of Li_2MnO_3 as a cathode material with better cycling performance predicted in high pressure synthesis

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Electronic Supplementary Information

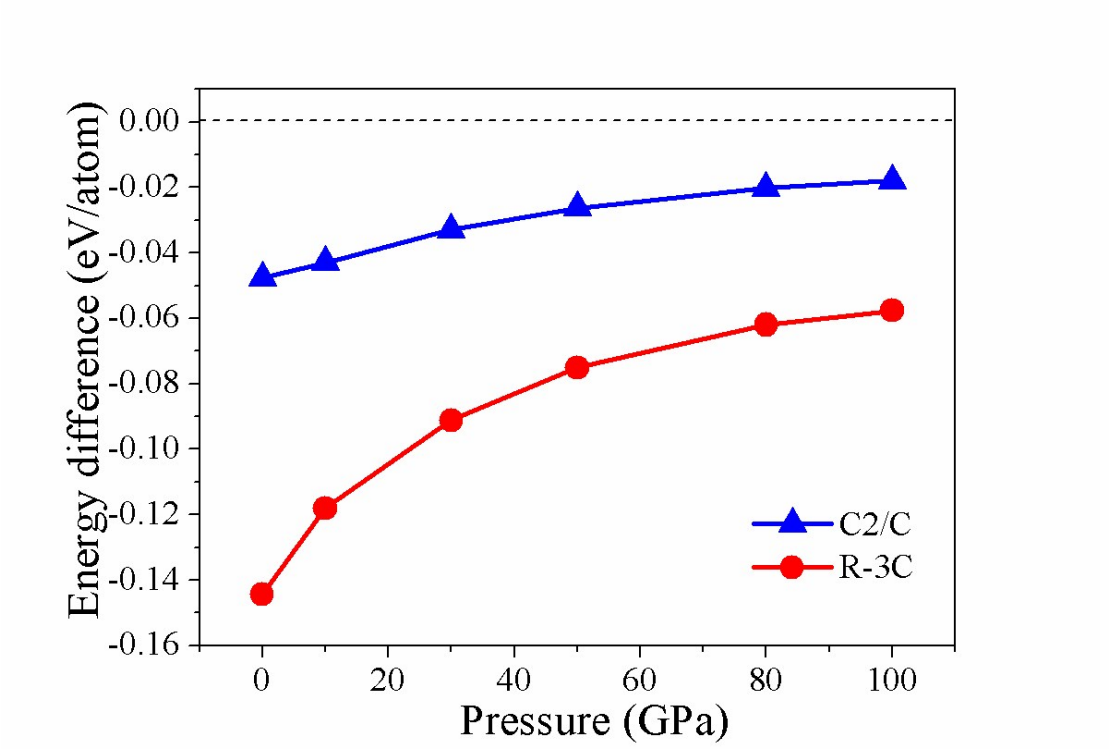

Figure S1. Pressure dependence of enthalpy curves of predicted structures with respect to the layer structure.

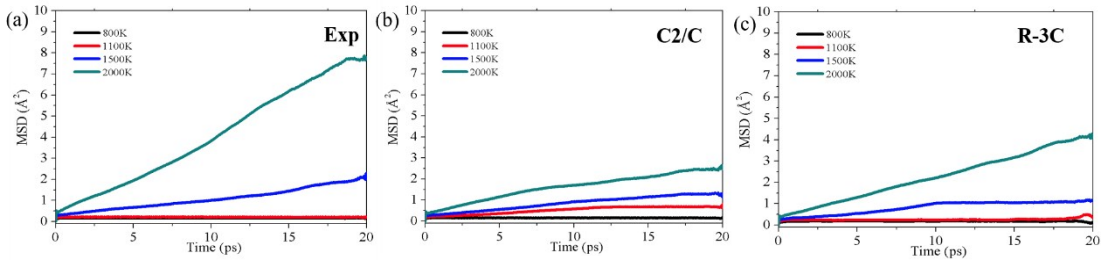

Figure S2. The MSD of Li as a function of time at different temperatures in 2×2×2 supercell with two Li vacancies for (a) experimental layer, (b)C2/C and (c) R-3C phase.

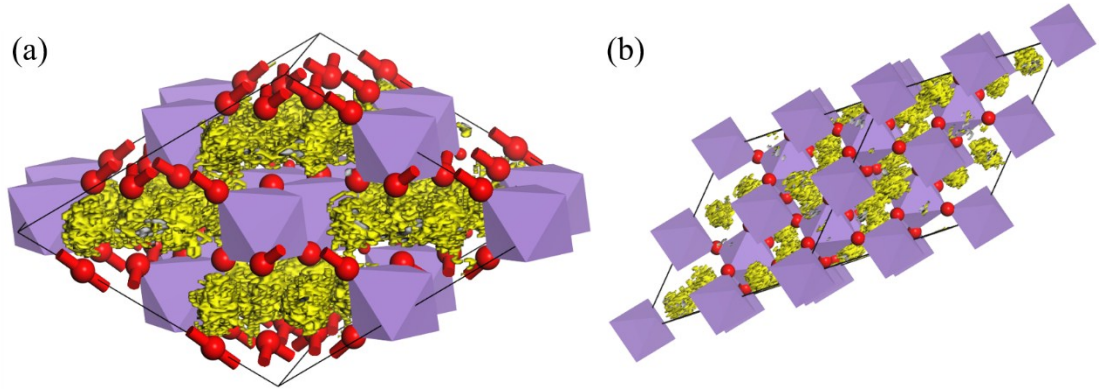

Figure S3. The projection (yellow) of Li trajectories in the fixed-volume 2 × 2 × 2 supercell at 2000 K for (a) C2/C, (b) R-3C. The O (red), Mn-O octerhedrons (purple polyhedrons) are labeled respectively.

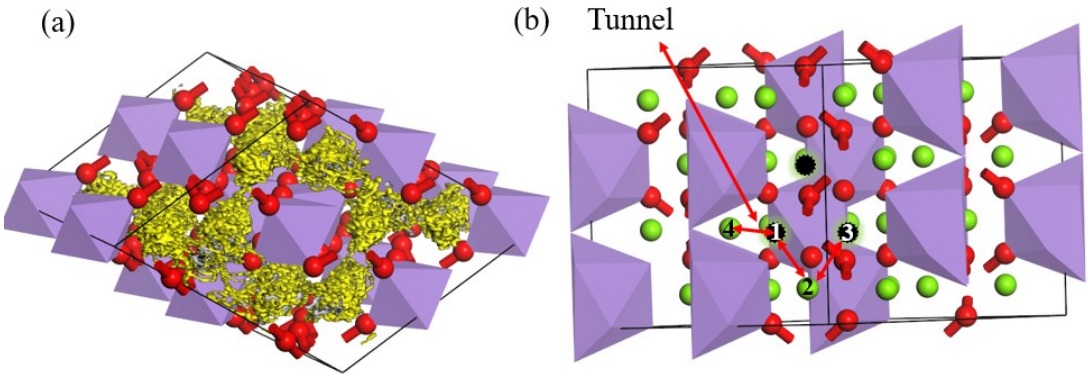

Figure S4. The projection (yellow) of Li trajectories for C2/C with high vacancy content (a) and ionic migratory schematic diagrams of tri-vacancies. The black ball represent the vacancies of Li atoms.