K-Gradient Doping to Stabilize Spinel Structure of $Li_{1.6}Mn_{1.6}O_4$ for Li^+ recovery

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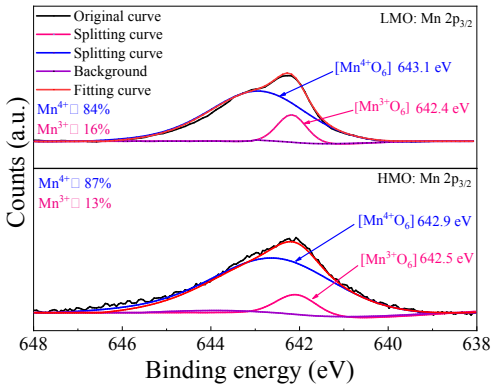

Fig. S1. The fitting curve of Mn 2p for undoped samples.

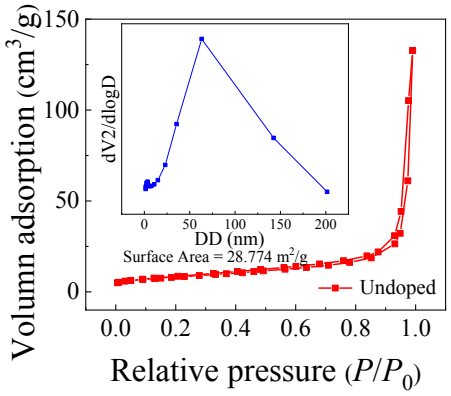

Fig. S2. Nitrogen ad/desorption isotherms and pore size distribution of HMO.

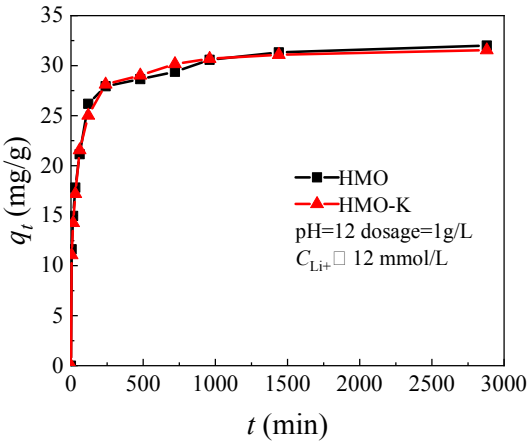

Fig. S3 The adsorption rate of HMO and HMO-K .

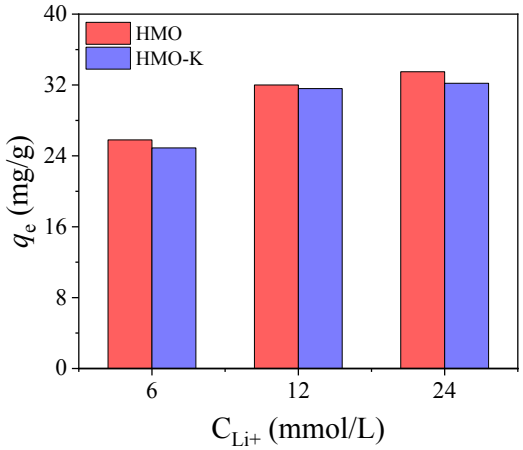

Fig. S4 Adsorption capacity of HMO and HMO-K at different initial Li^+ concentration.

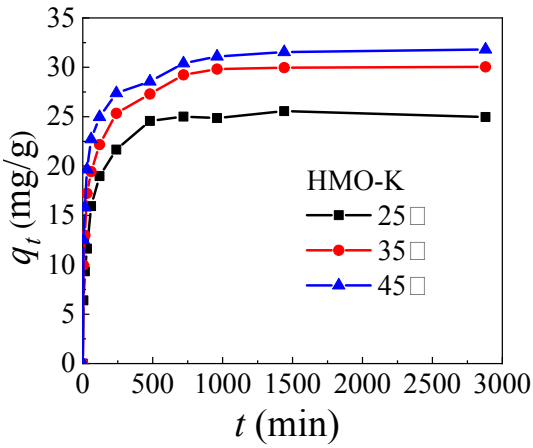

Fig. S5 Adsorption capacity of HMO-K at various temperature.

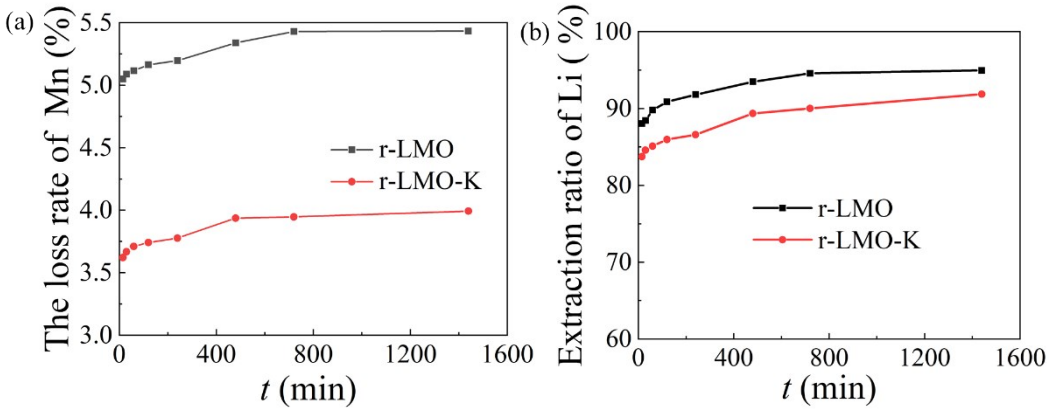

Fig. S6. (a) The Mn dissolution of r-LMO-K and r-LMO; (b) Li^+ extract of r-LMO-K and r-LMO.

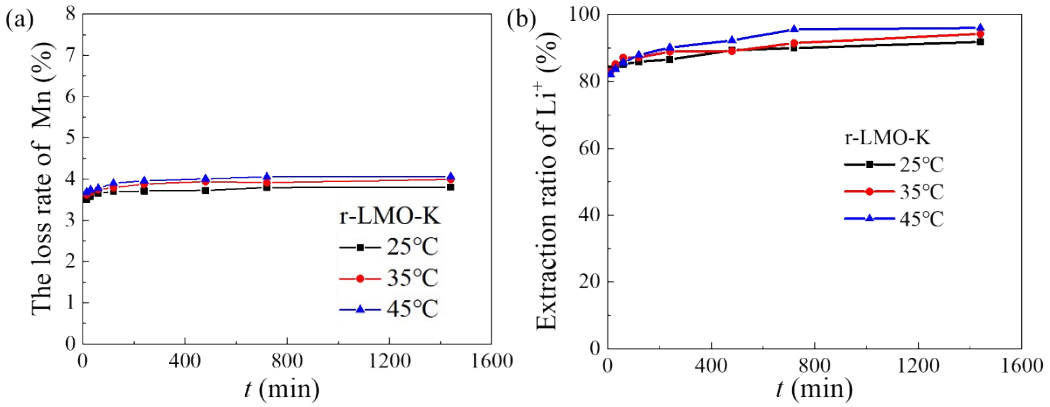

Fig. S7. The desorption properties in different temperature (C_{HCl} = 0.6 mol/L). (a) Dissolution of Mn and (b) desorption rate of Li^+.

First principles calculations

Density functional theory (DFT) [1, 2] calculations were implemented by the Vienna Ab-initio Simulation Package (VASP) with the projector-augmented wave (PAW) [3]method, and the Perdew-Burke-Ernzerh (PBE) exchange-correlation functional [4] of the Generalized Gradient Approximation (GGA) [5-7]. Owing to the strong-correlation d-electrons of Mn metals, the Hubbard-type U correction was adopted. In order to gain accurate computation, the U values of 4.5 eV [8] were used. The cutoff energy of 500 eV was adopted in all calculations. The thickness of the vacuum is set to the 15 Å. An appropriate k-point mesh of 6×6×6 and 3×3×1 for Bulk and the Li4Mn5O12 (100) surface was adopted, respectively. In order to improve the quality of DOS and charge, the k-point mesh of 4×4×1was adopted. The electronic total energies convergence criterion was set at 10–4 eV. The atomic positions were stable until Hellmann-Feynman forces on each atom were less than a threshold value of 0.01 eV.

References

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