Enhancing adsorption capacity and structural stability of $Li_{1.6}Mn_{1.6}O_4$ adsorbents by anion/cation co-doping

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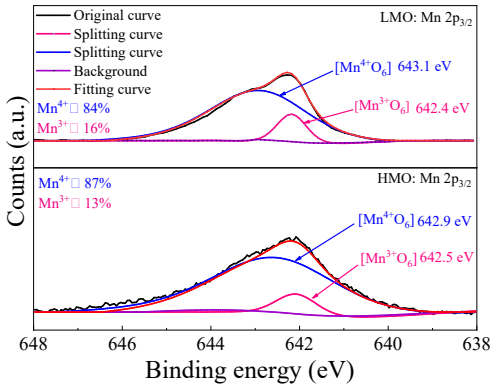

Fig. S1. The fitting curve of Mn $2p_{3/2}$ in the XPS spectra of the undoped samples of LMO and HMO.

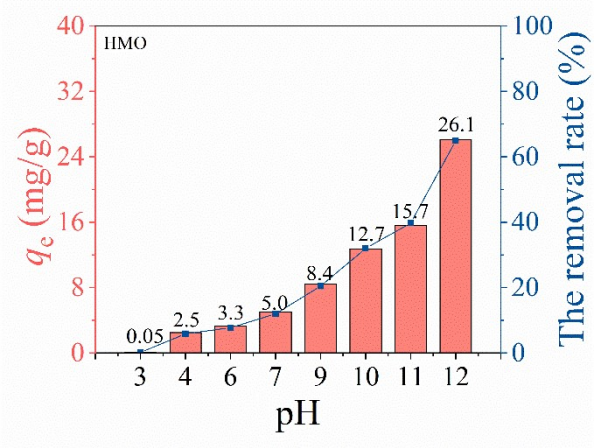

Fig. S2. The adsorption capacity and removal rate of HMO at various pH.

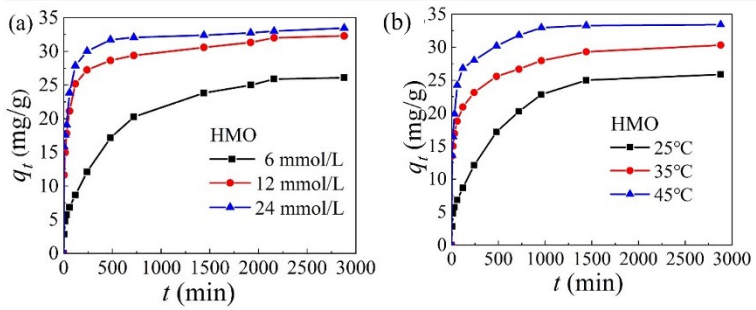

Fig. S3. The adsorption capacity of HMO: (a) various initial adsorption concentration, (b) various temperature .

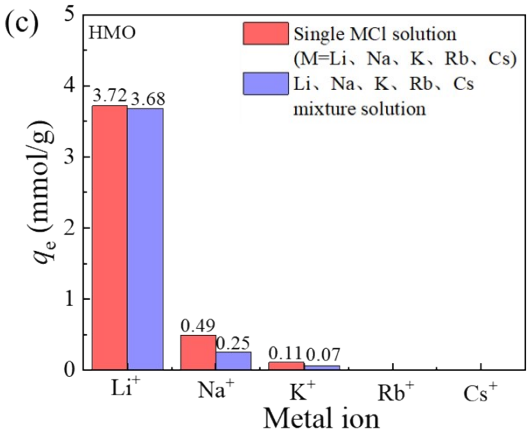

Fig. S4 The selectivity experiments of HMO.

Table S1 Contrast of adsorption capcaity in the present work with other works.

adsorbent	solution	C_{Li+} (mmol/L)	q_e (mg/g)	refs
$Li_{1.6}Al_xMn_{1.6-x}O$	LiOH	50	32.6	[9]
$Li_{1.6}Mn_{1.6-x}Cr_xO_4$	salt lake	32	31.67	[10]
$Li_{1.6}Mn_{1.6}O_4$	salt lake	38.3	27.15	[11]
$LiMn_2O_4$ foams	LiOH	345	20.9	[12]
$H_{1.6}Mn_{1.6}O_4$/PAN	LiCl/LiOH	5	10.3	[13]
HMO/Al_2O_3	seawater	4.3	6.2	[14]
HMO-Al-5%	LiCl	6	29.9	[15]
HMO-SAl	LiCl	6	33.7	This work

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.

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