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$LiCr(MoO_4)_2$: a New High Specific Capacity Cathode Material for Lithium Ion Batteries

Kai Feng[†], Fuxiang Wang[†], Xin Yang[†], Hongzhang Zhang[‡§]*, Xianfeng Li[‡§]*, Huamin Zhang[‡§]

[†]Shandong Collaborative Innovation Center of Light Hydrocarbon Transformation and Utilization, College of Chemistry & Engineering, Yantai University, Yantai, 264005, China

[‡]Division of energy storage, Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Zhongshan Road 457, Dalian, 116023, China.

[§]Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), Dalian 116023 (P.R. China)

The diffusion coefficient of Li ions (D) is calculated according to the following Equation (1) and Equation (2)

$D=R^2T^2/2A^2n^4F^4C^2\sigma^2$ （1）

$Z'=R_s+R_{ct}+\sigma\omega^{-1/2}$ （2）

where R is the gas constant, T is the absolute temperature, A is the surface area of the cathode, n is the number of electrons per molecule during oxidization, F is the Faraday constant, C is the concentration of lithium-ion, σ is the Warburg factor which has a relationship with Z' as shown in Eq. (2), R_s is the resistance between the electrolyte and electrode, R_{ct} is the charge transfer resistance, and ω is angle frequency. The constant phase element (CPE) stands for the double layer capacitance. The charge transfer resistance estimated from the semicircle in upper-middle frequency region is associated with the charge transfer process. And the numerical value of the diameter of the semicircle on the Z' axis is approximated to be the charge transfer resistance (Rct).

Table S1 Kinetic parameters of $LiCr(MoO_4)_2$@C.

Sample	R_{ct} (Ω)[(a)]	σ [(b)]	D_{Li^+} ($cm^2\ s^{-1}$) [(c)]
$LiCr(MoO_4)_2$@C	90	198	8.1×10^{-17}

[(a)] R_{ct}: charge transfer resistance [(b)]σ: Warburg factor [(c)]D_{Li^+}: diffusion coefficient of Li^+ion

Figure S1 (a) Crysta structure of $LiCr(MoO_4)_2$, (b) BVS-DMs of of $LiCr(MoO_4)_2$.

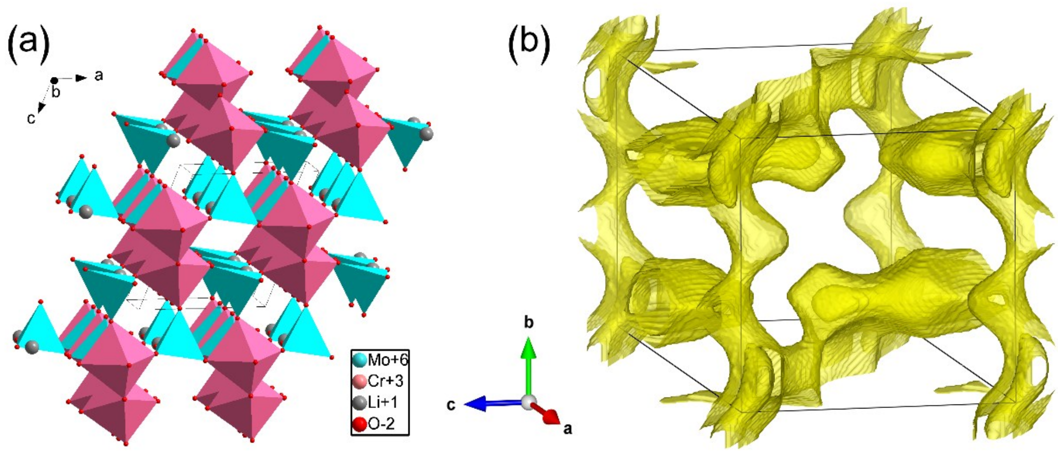

Figure S2 SEM of $LiCr(MoO_4)_2$.