**Supplementary Information**

**MOF-derived molybdenum selenide on Ti3C2T*x*** **with superior capacitive performance for lithium-ion capacitors**

*Jianjian Zhong*1), *Lu Qin*1), *Jianling Li*1), 🖂, *Zhe Yang*1), *Kai Yang*2), *and* *Mingjie Zhang*2)

1) State Key Laboratory of Advanced Metallurgy, University of Science and Technology Beijing, Beijing 100083, China

2) State Key Laboratory of Operation and Control of Renewable Energy and Storage Systems, China Electric Power Research Institute, Beijing 100192, China

**🖂**Corresponding Authors: Jianling Li E-mail: lijianling@ustb.edu.cn



**Figure S1.** The XPS full spectra of Ti3C2Tx and Ti3C2Tx@MoSe2.



**Figure S2.** The high-resolution XPS spectra of (a and c) O 1s and (b and d) C 1s for Ti3C2Tx and Ti3C2Tx@MoSe2, respectively.

**Figure S2a and c** show the XPS spectra of O 1s for the two samples. Both the materials possess the characteristic peaks of Ti-O, C-Ti-OH bonds and Ads H2O. But the O 1s spectrum displays a peak at 530.7 eV indexed to Mo-O bond (which is different from the peak at 531.4 eV of C-Ti-O for Ti3C2Tx indicating the successful growth of MoSe2 on the surface. And **Figure S2d** shows the characteristic peak of C-Se bond at 287.0 eV instead of C-O bond, which maybe because the residual selenium not involved in the reaction and stronger interaction of C-Se than Mo-Se enable the residual Se powders to bond with C atoms preferentially.



**Figure S3.** The spectra of (a) Ti 2p and (b) Se 3d at different potentials of Ti3C2Tx@MoSe2 during the first cycle.

The Ti 2p spectrum in **Figure S3a** during the initial charge-discharge depicts that the peaks at 458.5 and 464.1 eV assigned to Ti-Se bond gradually disappear during the discharging, which maybe result from the reduction of Se2– (corresponding to the Se 3d spectrum) changing the surrounding environment of Ti-Se bond. Then the peak of Ti-Se bond dose not return to original state during charging which is attributed to the de-lithiation of Li2Se to elemental selenium not binding with Ti element.



**Figure S4.** The (a and b) charge and discharge curves of different cycles and (c and d) corresponding differential capacity curves at the current density of 300 mA g–1 of Ti3C2Tx and Ti3C2Tx@MoSe2, respectively.



**Figure S5.** (a and c) The schematic illustration of a single step randomly selected from the charge-discharge for Ti3C2Tx and Ti3C2Tx@MoSe2, respectively. (b and d) The linear relationship between E and τ1/2 during the impulse corresponding to (a) and (c).

GITT is regarded as a standard method for the determination of Li+ diffusion on account of the elimination of ohmic drop which is inevitable in other methods.[1] A single step selected randomly from the GITT curves of Ti3C2Tx and Ti3C2Tx@MoSe2 are shown in **Figure S5 a and c**, respectively. The single step illustrates the principle that apply a constant current to the electrode for a certain period of time, then record and analyze the potential responding curve after current pulse. A constant current *I*0 is applied to the electrode at equilibrium potential *E*0 at time *t*0, which arises the diffusion of Li+ at electrode surface to produce a concentration gradient with the variation of potential. The current is suspended after an elapsed time of *τ* and Li+ inside electrode achieve the equilibrium concentration with a new equilibrium potential *E*1 via diffusion. The formula of Li+ diffusion coefficient in a thin film electrode is as follows:[1]

$$\tilde{D}\_{Li}=\frac{4}{πτ}\left(\frac{m\_{B}V\_{m}}{M\_{B}S}\right)^{2}\left(\frac{∆E\_{s}}{∆E\_{t}}\right)^{2} \left(τ\leq {L^{2}}/{\tilde{D}\_{Li}}\right)$$

where *m*B, *M*B, *V*m, *S* represent the mass atomic weight, molar volume (can be calculated by the volume of the crystal unit cell) and the surface area of the electrode material, respectively, Δ*E*s is the variation of the equilibrium potential, and Δ*E*t represents the variation of transient voltage within the pulse time *τ*.

And the linear relationship of *E* and *τ*1/2 is plotted in **Figure S5 b and d**,which demonstrates the feasibility of the Galvanostatic Intermittent Titration Technique and the rationality to adopt above formula to calculate the diffusion coefficient *D*Li+.



**Figure S6.** The CV curves for (a) Ti3C2Tx and (b) Ti3C2Tx@MoSe2 at the sweep rates from 5.0 to 20 mV s–1.



**Figure S7.** The electrochemical performance of activate carbon (AC): (a) CV curves between 2.0-4.0 V, (b) rate performance from 30 to 1500 mA g–1, (c and d) cycle performance at 750 and 1500 mA g–1, respectively.

**Reference**

[1] W. Weppner and R. A. Huggins, Determination of the kinetic parameters of mixed‐conducting electrodes and application to the system Li3Sb. J. Electrochem. Soc., 124(1977), p. 1569-1578.