Supplementary Material

MoS_2 nanosheets coupled on $Ti_3C_2T_x$ prepared by molten salt etching for enhancing lithium storage performance

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Materials Characterization

The structure and phase purity of the synthesized materials were assessed through X-ray diffraction (XRD) employing Cu Kα radiation. The morphological details, grain size, and microstructure of the materials were examined using scanning electron microscopy (SEM, SU 8020, Hitachi), transmission electron microscopy (TEM, Tecnai G2F20), and high-resolution TEM (HR-TEM). X-ray photoelectron spectroscopy (XPS) analysis was conducted using a Thermo Scientific ESCALAB 250 with Al Kα as the excitation source.

Electrochemical measurements

The electrochemical performance of the as-prepared materials was evaluated using CR2032 coin-type cells where Li foil served as the counter electrode. The working electrode was fabricated by mixing the as-prepared material, acetylene carbon black, and polyvinylidene fluoride (PVDF) in a weight ratio of 8:1:1 in a certain amount of N-Methylpyrrolidone (NMP). The uniformly mixed slurry was spread on a Cu foil and dried at 80 ℃ for 12 h under vacuum. The coating thickness of materials is about 100 μm. The assembly of the coin cells was carried out in an argon-filled glove box using polypropylene membrane (Celgard 2400) as the separator and 1 M $LiPF_6$ dissolved in an organic solvent with EC/DMC/EMC = 1:1:1 as the electrolyte. The charge and discharge measurements were carried out on a LAND-CT2001C test system at different current densities. Cyclic voltammogram experiments were performed on an Autolab PGSTAT302N electrochemical workstation at various scan rates.

Density functional theory (DFT) simulations

The simulations were performed using the Density Functional Theory (DFT) implemented in the Cambridge Sequential Total Energy Package (CASTEP). The Perdew-Burke-Ernzerhof (PBE) exchange-correlation function of the generalized gradient approximation (GGA) was employed for calculations, and ultrasoft pseudopotentials were used for ion-electron interactions. The energy cutoff was set to 500 eV to achieve energy convergence down to 1×10^{-5} eV. The Brillouin zone was sampled using the Monkhorst-Pack method. For diffusion pathway calculations, the transition state search method was applied, including complete linear synchronous transit and quadratic synchronous methods. The atomic structures and electron density differences were visualized using VESTA.

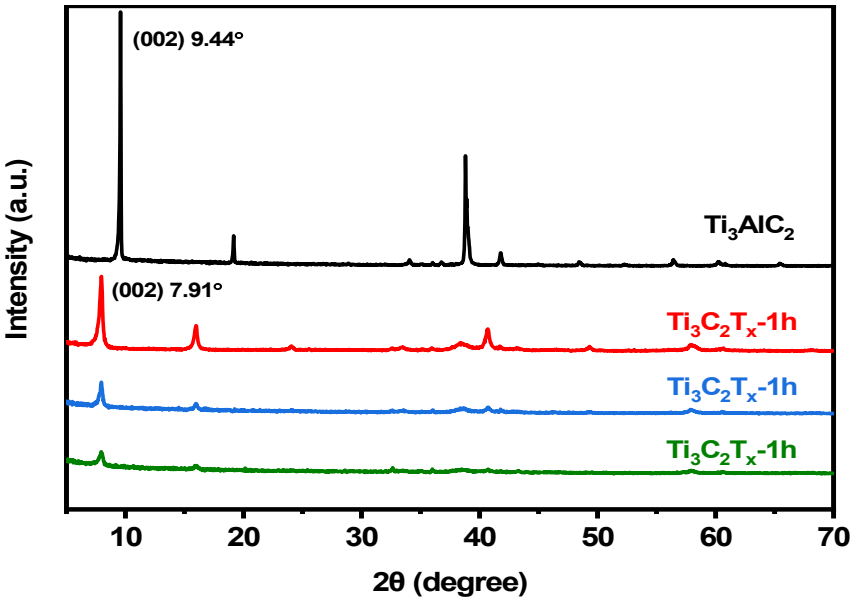

Fig. S1. XRD of Ti_3AlC_2 and $Ti_3C_2T_x$

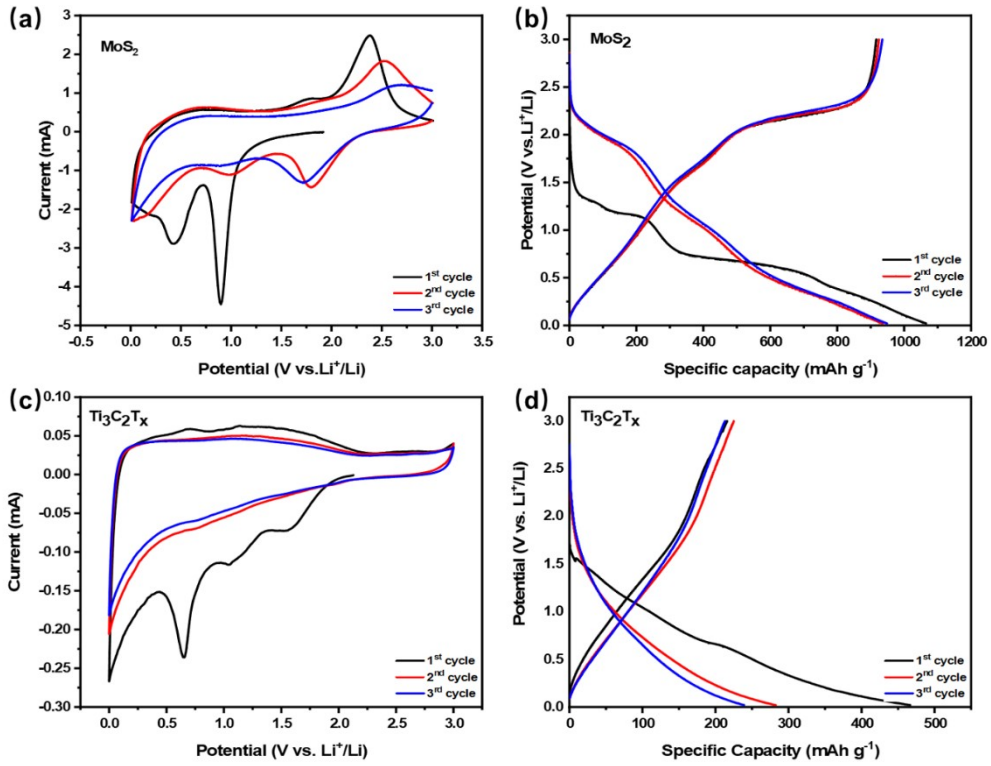

Fig. S2. CV curves of (a) MoS_2 and (c)$Ti_3C_2T_x$; Charge and discharge curves of (b) MoS_2 and (d)$Ti_3C_2T_x$

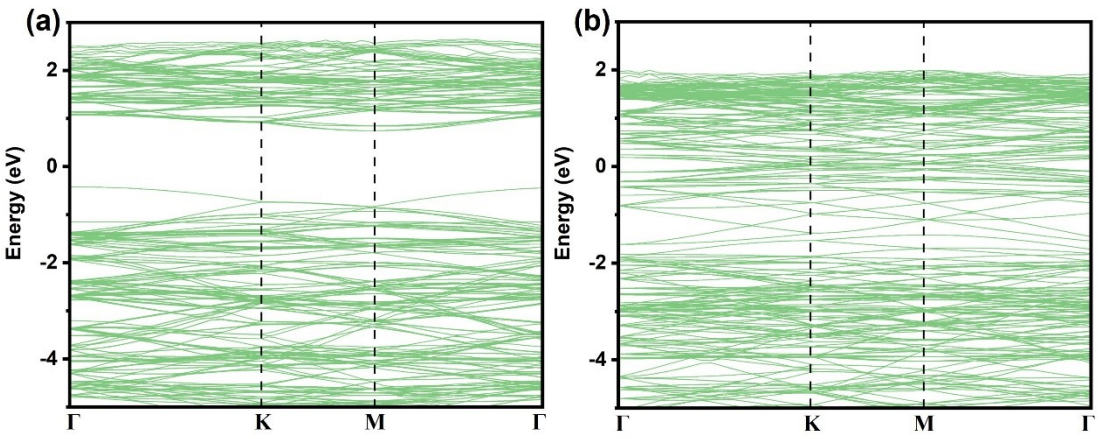

Fig. S3. Band curves of (a) MoS_2 and (b) $MoS_2/Ti_3C_2T_x$

Table. S1. A comparison of the cycling performance of $MoS_2/Ti_3C_2T_x$ with the recently reported MoS_2 anode materials for Li-ion batteries in other literature.

Materials	Capacity ($mAh \cdot g^{-1}$)	Density ($mA \cdot g^{-1}$)	Cycles	Ref.
$MoS_2/Ti_3C_2T_x$	460.6	100	100	This work
Exfoliated MoS_2 nanosheets	385	100	100	[1]
N-doped carbon nanofiber@MoS_2 nanosheets	495	100	100	[2]
MoS_2 nanosheets aligned on carbon paper	286	100	80	[3]
MoS_2/graphene	573	100	50	[4]
f-MoS_2/C-3	307	500	50	[5]

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