Supplementary material for

Crystal Water Intercalated Interlayer Expanded MoS_2 Nanosheets as Cathode for Efficient Zinc-Ion Storage

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Calculation details

(i) ***Segregation of Capacitive and Diffusive parts from CV:***

To evaluate the charge storage mechanism of ZIBs, current (i) and scan rate (v) is analyzed from the CV curve by using the following reaction:

$$i = av^b \tag{S1}$$

Here a and b are variable parameters. The value of b can be calculated by the slope of log i versus log v plot, which provides the charge storage kinetics. If the value of b is 1, the capacitive process is dominating, while the diffusive process is dominating when b is 0.5. For segregating the capacitive and diffusive currents, the following formula is used.

$$i(V) = a_1 v + a_2 v^{\frac{1}{2}} \tag{S2}$$

Here i and v are the current and scan rates. The values of a_1 and a_2 are calculated by finding the slope and intercept of the $i(V)/v^{1/2}$ versus the $v^{1/2}$ plot.

(ii) Calculation of diffusion co-efficient from GITT:

For GITT studies, the cell was charged/discharged for 8 mins and rested for 32 mins. The diffusion coefficient of Zn-ions (D_{Zn}) can be calculated by the following equation:

$$D_{Zn} = \frac{4}{\pi\tau}\left(\frac{m_B V_M}{M_B A}\right)^2 \left(\frac{\Delta E_s}{\Delta E_\tau}\right)^2 \tag{S3}$$

Here, τ is the time of charging/discharging (s), m_B is the active mass loading (g), V_M is the molar volume of MoS_2 (cm^3/mol), M_B is the molecular weight of MoS_2 (g/mol) and A is the electrode/electrolyte contact area (cm^2). Moreover, ΔE_τ and ΔE_S are the variations of cell voltage and steady-state voltage, respectively.

(iii) Calculation of diffusion co-efficient from EIS:

D_{Zn} can also be calculated using EIS spectra by using the equation S4. In the equation, R represents the gas constant (8.314 J/mol/K), T represents the absolute temperature (-273.15 K), A is the electrode/electrolyte contact area (cm^2), n is the number of electrons transferred during the electrochemical process (1.18 in this system), F is the Faraday constant (96500 C/mol), C is the concentration of Zn (calculated to be 1.84×10^{-2} mol/cm^3), and σ is the Warburg factor (slope of Z′ vs. $\omega^{-1/2}$ plot)

$$D_{Zn} = \frac{R^2T^2}{2A^2n^4F^4C^2\sigma^2} \quad \text{(S4)}$$

(iv) Calculation of Zn-ions concentration:

Unit cell volume of MoS_2 is determined by "a (3.16 Å) × b (3.16 Å) × c (12.29 Å) × sin120° = 106.28×10^{-24} cm^3". 1 cm^3 of MoS_2 have $1/106.28 \times 10^{-24} = 9.41 \times 10^{21}$ unit cells. In our case, ZIB shows the maximum specific capacity of 197 mAh/g, which signifies 0.59 Zn^{2+} insertion in MoS_2 ($Zn_{0.59}MoS_2$). Each molecule of MoS_2 has 0.59 Zn ions and each unit cell contains 2 molecules. Therefore, 1 cm^3 has $(9.41 \times 1021/6.02 \times 1023) \times 2 \times 0.59 = 1.84 \times 10^{-2}$ mol Zn-ions.

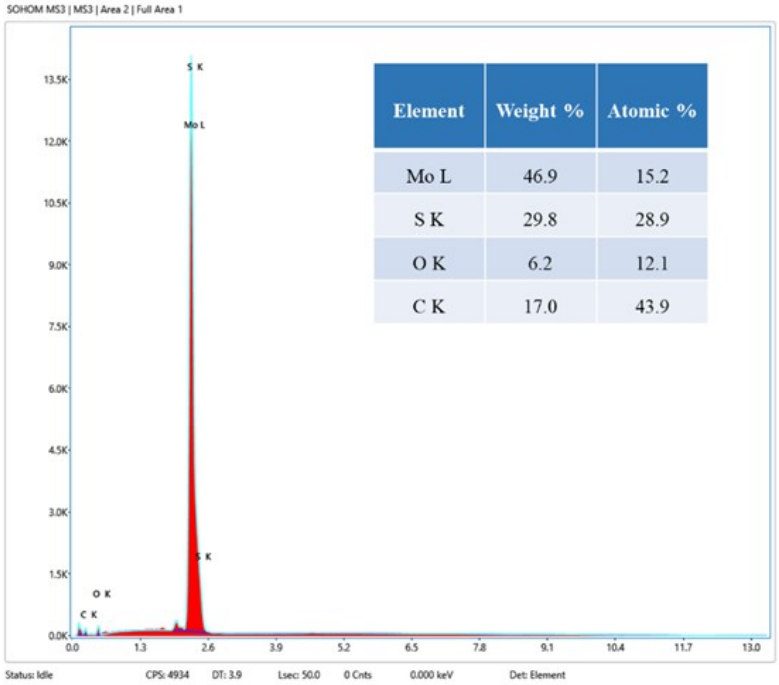

Figure S1: EDX spectra of the synthesized MoS_2 nanostructures

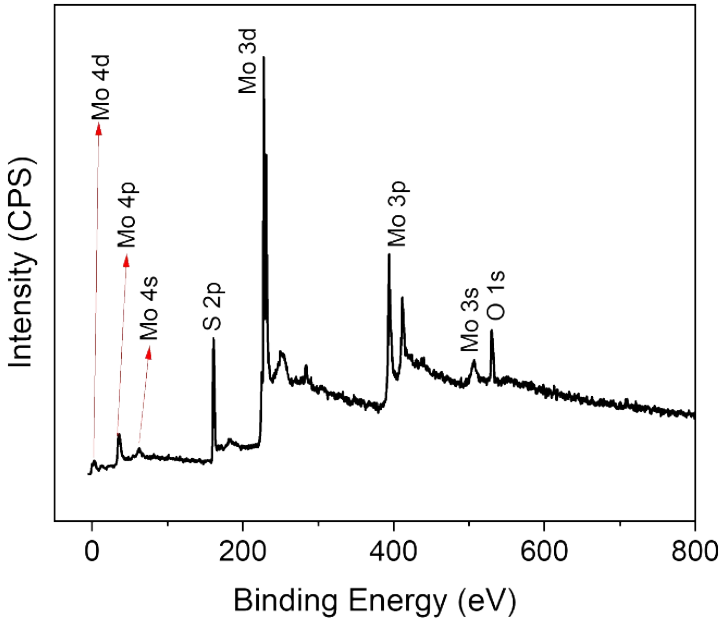

Figure S2: XPS survey spectra of the as-synthesized water intercalated MoS_2 nanostructures

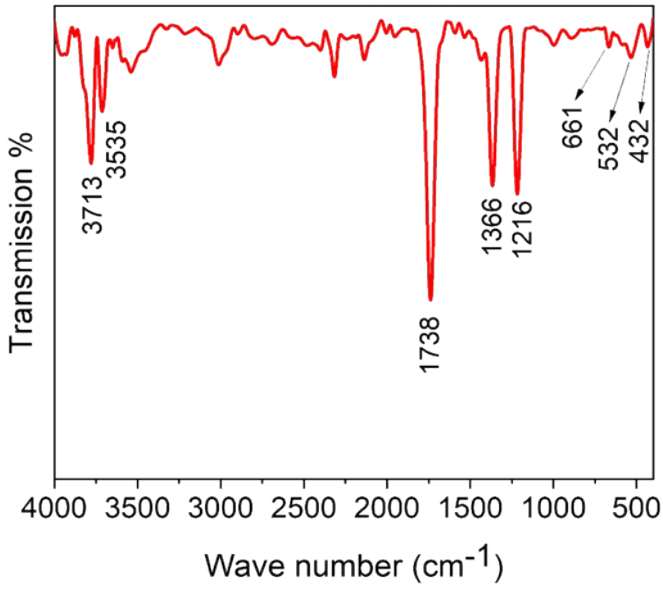

Figure S3: FTIR spectra of the synthesized MoS_2 nanostructures

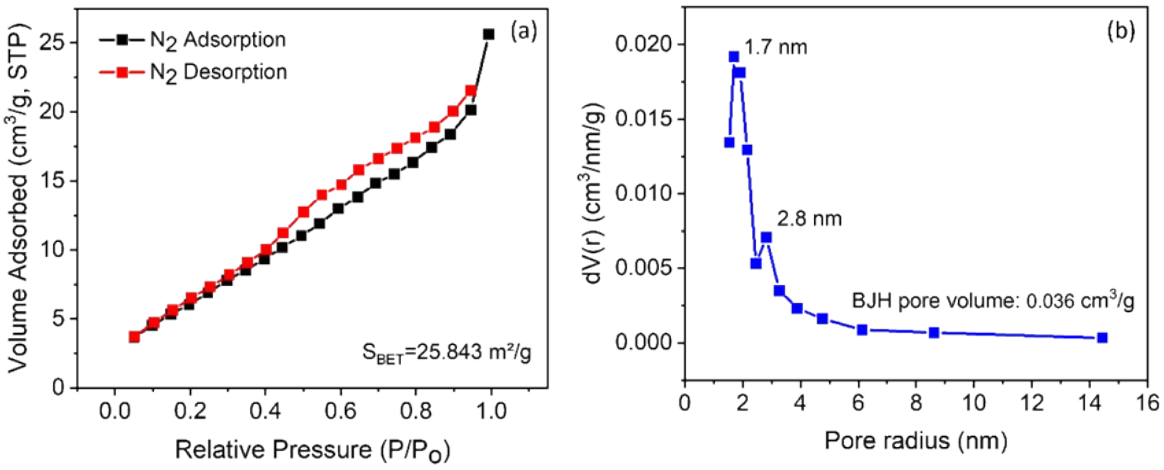

Figure S4: (a) N_2 adsorption-desorption isotherm and (b) BJH pore-size distribution plots of the MoS_2 nanosheets

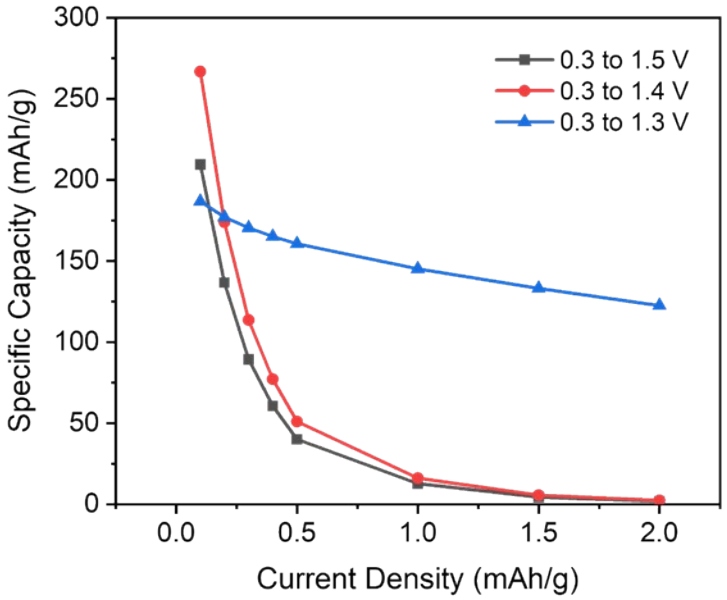

Figure S5: Specific capacity of the MoS_2 sample at different potential windows

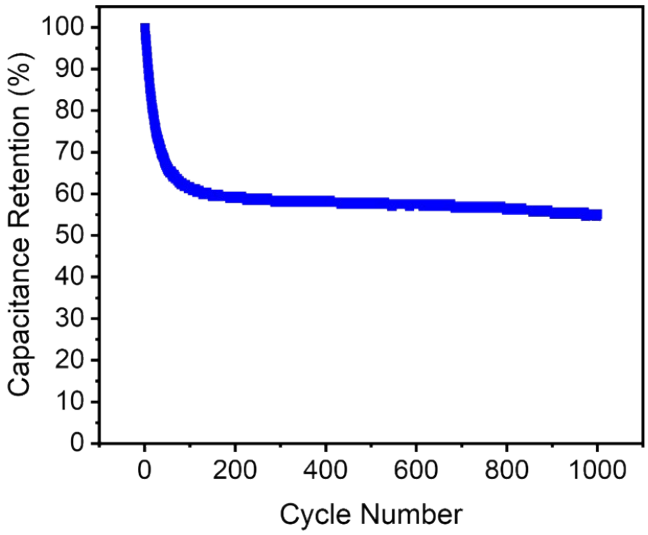

Figure S6: Cycling study of MoS_2 nanostructures for 1000 GCD cycles measured at 2 A/g

Table S1: Some key literature on MoS_2-based cathode materials for ZIBs

S. No.	Cathode Material	Interlayer Spacing	Electrolyte	Voltage	Specific Capacity	Cyclic Retention	Ref.
1	MoS_2	-	2 M $ZnSO_4$	0.1-2 V	18 mAh/g at 0.05 A/g	-	[1]
2	MoS_2	7.3 Å	2 M $ZnSO_4$	0.3-1.5 V	202.6 mAh/g at 0.1 A/g	98.6% after 600 cycles	[2]
3	MoS_2 (~70% 1T)	-	3 M $Zn(CF_3SO_3)_2$	0.25–1.25 V	168 mAh/g at 0.1 A/g	98.1% after 400 cycles	[3]
4	MoS_{2-x} (S-vacancy)	6.86 Å	3 M $Zn(CF_3SO_3)_2$	0.25–1.25 V	138.6 mAh/g at 0.1 A/g	87.8% after 1000 cycles	[4]
5	N-MoS_2	8.6 Å	3 M $Zn(CF_3SO_3)_2$	0.2-1.3 V	149.6 mAh/g at 0.1 A/g	89.1% after 1000 cycles	[5]
6	1T MoS_2@CC	6.7 Å	3 M $Zn(CF_3SO_3)_2$	0.25–1.25 V	198 mAh/g at 0.1 A/g	87.8% after 2000 cycles	[6]
7	MoS_2/CTAB	10 Å	3 M $ZnSO_4$	0.2-1.3 V	181.8 mA/g at 0.1 A/g	~92.8% after 2100 cycles	[7]
8	MoS_2-H_2O	9.1 Å	3 M $Zn(CF_3SO_3)_2$	0.25-1.25	164.1 mAh/g at 0.1 A/g	83.1% after 100 cycles	[8]
9	MWCNTs@amorphous carbon@MoS_2	8.8 Å	3 M PVA-$Zn(CF_3SO_3)_2$	0.13-1.2 V	181 mAh/g at 0.1 A/g	78% after 1000 cycles	[9]
10	**Crystal water intercalated MoS_2**	**7.9 Å**	**2 M $ZnSO_4$**	**0.3-1.3 V**	**197 mAh/g at 0.1 A/g**	**55% after 1000 cycles**	**This work**

References

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