Supplementary Information

Boosting magnesium storage in MoS₂ via 1T phase introduction and

interlayer expansion strategy: Theoretical prediction and experimental

verification

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Fig. S1. N₂ adsorption-desorption patterns of (a) the interlayer-expanded 1T/2H MoS₂ nanosheets and

(b) the pure 2H MoS₂ nanosheets.



Fig. S2. (a) SEM, (b) TEM, (c) SAED patterns, (d) HADDF image and (e-f) EDS mapping of 2H MoS_2

nanosheets.



Fig. S3. (a)EIS of a SS//0.4 M APC//SS cell using glass fiber separator. (b) The chronoamperometry profiles of Mg//0.4 M APC//Mg cell using glass fiber separator, and the corresponding EISs before and after polarization (shown in insets).



Fig. S4. The deconvoluted XPS results of high resolution (a) Mo3d spectrum and (b) S2p spectrum of the synthesized MoS_2 electrode after 50 cycles.



Fig. S5. *Ex-situ* HRTEM images of the 1T/2H MoS₂ electrode in MIBs: (a) First discharged sample, (b) First charged state sample, (c) Second discharged sample, (d) Second charged state sample.



Fig. S6. STEM-HAADF image and EDS mapping of (a) discharged 1T/2H MoS₂ electrode and (b) charged 1T/2H MoS₂ electrode. EDS results of 1T/2H MoS₂ electrode in MIBs at (c) discharged stage from area #1 and (d) charged stage from area #2.



Fig. S7. Ex-situ XRD patterns of 1T/2H MoS₂ electrode in RMBs.



Fig. S8. Surface SEM images of the Mg anode after different discharge-charge cycles: (a) 1cycle, (b) 50

cycles, (d) 500 cycles.

 Table S1 The interlayer spacing size of different layerd transition metal sulfide for cathode of Mg batteries.

| Candidates | Interlayer spacing size | Ref. |
|-----------------------------------|-------------------------|-----------|
| Interlayer expanded $1T/2H MoS_2$ | 0.92 nm | This work |
| MoS ₂ | 0.62 nm | 66 |
| Interlayer expanded VS_2 | 1.00 nm | 67 |
| VS ₂ | 0.57 nm | 65 |
| WS ₂ | 0.62 nm | 70 |
| TiS ₂ | 0.57 nm | 68 |
| FePS ₃ | 0.64 nm | 69 |