Supporting Information

Lithium and Magnesium Storage Mechanism of Novel Hexagonal $NbSe_2$

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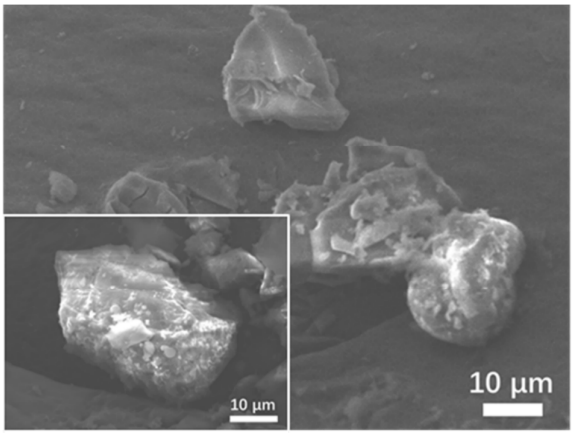

Figure S1. SEM image of $NbSe_2$ bulk.

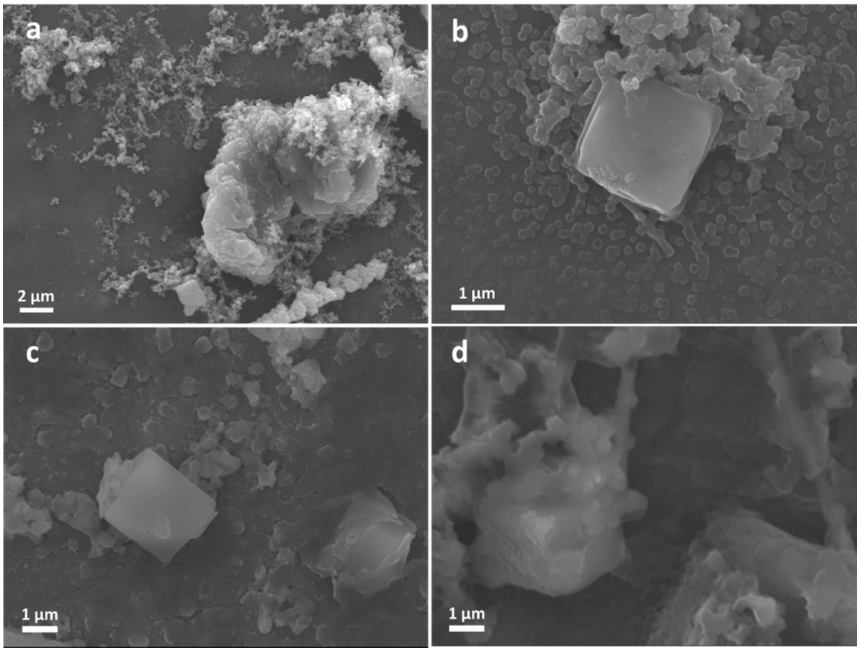

Figure S2. *Ex-situ* SEM of $NbSe_2$-M at different states for LIBs. (a) Initial, (b-c) discharged to 1.65 V and 0.01 V in the first cycle and (d) charged to 3 V in the second cycle.

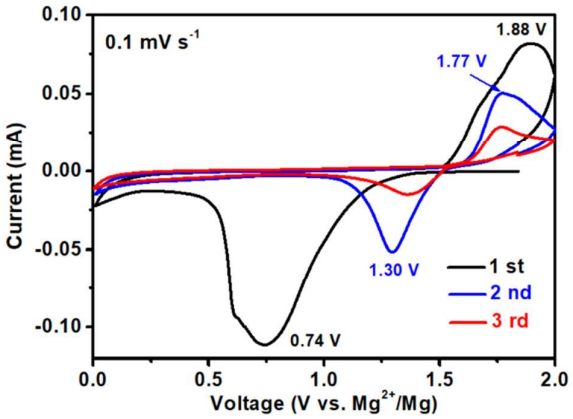

Figure S3. CV curves of initial three cycles under the scan rate of 0.1 mV s^{-1} of $NbSe_2$-M for MIBs.

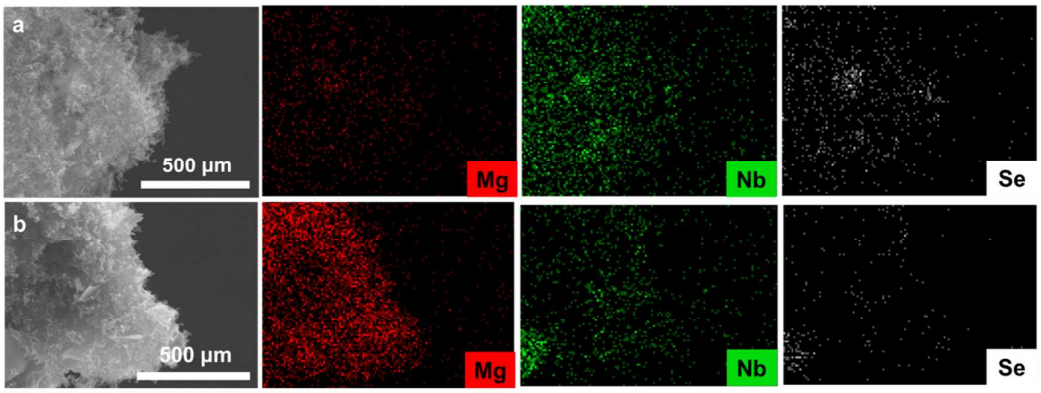

Figure S4. EDS mappings of Mg, Nb and Se elements in $NbSe_2$-M for MIBs before (a) and after (b) the GCD test.

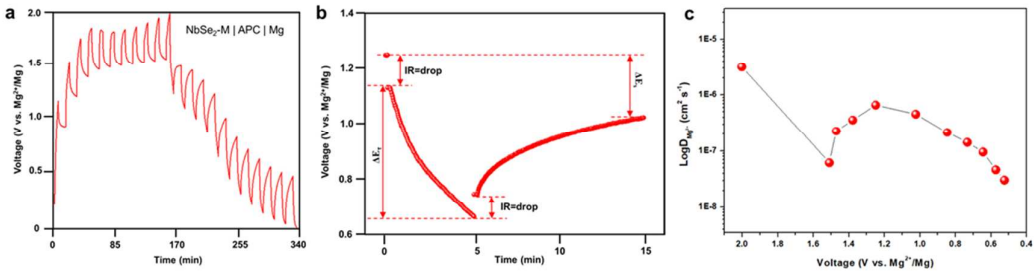

Figure S5. (a) GITT curves of $NbSe_2$-M in MIBs; (b) demonstration of a single titration during the GITT measurement; (c) diffusivity coefficient of Mg^{2+} ions in the $NbSe_2$-M at

different discharge state.

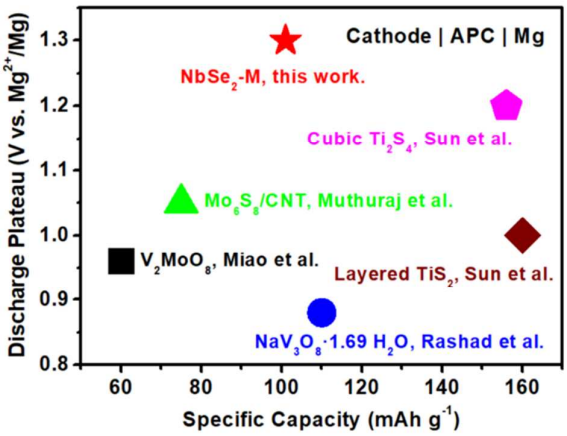

Figure S6. Comparison of the reported cathode materials in discharge plateau versus specific capacity for coin-type MIBs with APC as electrolyte and Mg metal as anode.

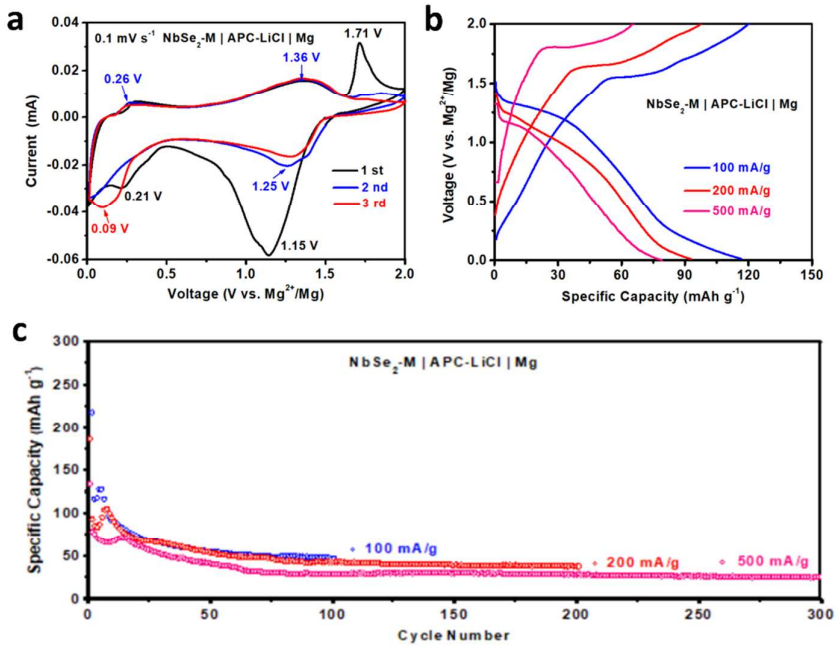

Figure S7. Electrochemical performance of $NbSe_2$-M for MLHBs. (a) CV curves under the scan rate of 0.1 mV s^{-1}. (b) GCD profiles at different current densities in the voltage

window of 0.01-2 V. (c) Cycling performances.

Table S1. Differences between H-$NbSe_2$ and H′-$NbSe_2$.

	H-$NbSe_2$	H′-$NbSe_2$
Reference code	**01-072-0864**	**01-089-5314**
Crystal system	**Hexagonal**	**Hexagonal**
Space group	**P63/mmc**	**P-6m2**
Space group number	**194**	**187**
a, b, c (Å)	**3.4446/3.4446/12.5444**	**3.4440/3.4440/25.2300**

Table S2. Comparison of the reported cathode materials in specific capacity and discharge plateau for coin-type MIBs with APC as electrolyte and Mg metal as the anode.

Cathode materials	Voltage window (V)	Current density (mA g^{-1})	Discharged capacity (mAh g^{-1})	Discharge plateau (V)	Specific energy density (Wh kg^{-1})	Journal/Ref.
Cubic Ti_2S_4	0.5-1.8	4.8	130	1.2	156	Energy Environ. Sci. [1]
	0.5-1.8	12	200 (60°C)	1.2	240	
Layered TiS_2	0.4-1.8	12	160 (60°C)	1	160	ACS Energy Lett. [2]
Interlayer-Expanded MoS_2	0.2-2	5	85	No Plateau	-	Nano Lett. [3]
V_2MoO_8	0.5-2.4	20	60	0.96	57.6	Nano Energy [4]
$NaV_3O_8 \cdot 1.69\ H_2O$	0.05-2	10	110	0.88	96.8	ACS Appl. Mater. Inter. [5]
Bronze TiO_2	0.01-2	20	45	No Plateau	-	J. Power Sources [6]
Mo_6S_8/CNT	0.5-2	60	75	1.05 (main)/1.14	78.8	Mater. Res. Bull. [7]
$NbSe_2$-M	0.01-2	200	101	1.30	131.1	This work

References

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