Supporting Information

Exfoliated Graphene Oxide/MoO$_2$ Composites as Anode Materials in Li Ion Batteries: An Insight into Intercalation of Li and Conversion Mechanism of MoO$_2$

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[*]Corresponding author. Tel: +65 6516 2605; E-mail address: phymvvr@nus.edu.sg; msemvvr@nus.edu.sg; reddymvvr@gmail.com (M. V. Reddy).
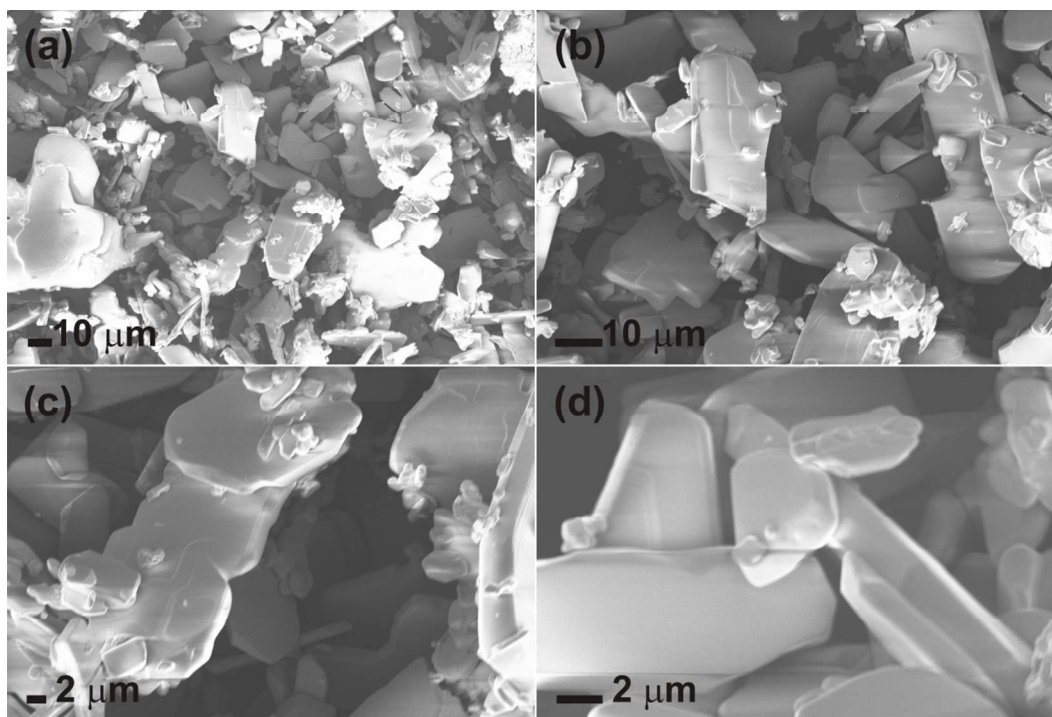
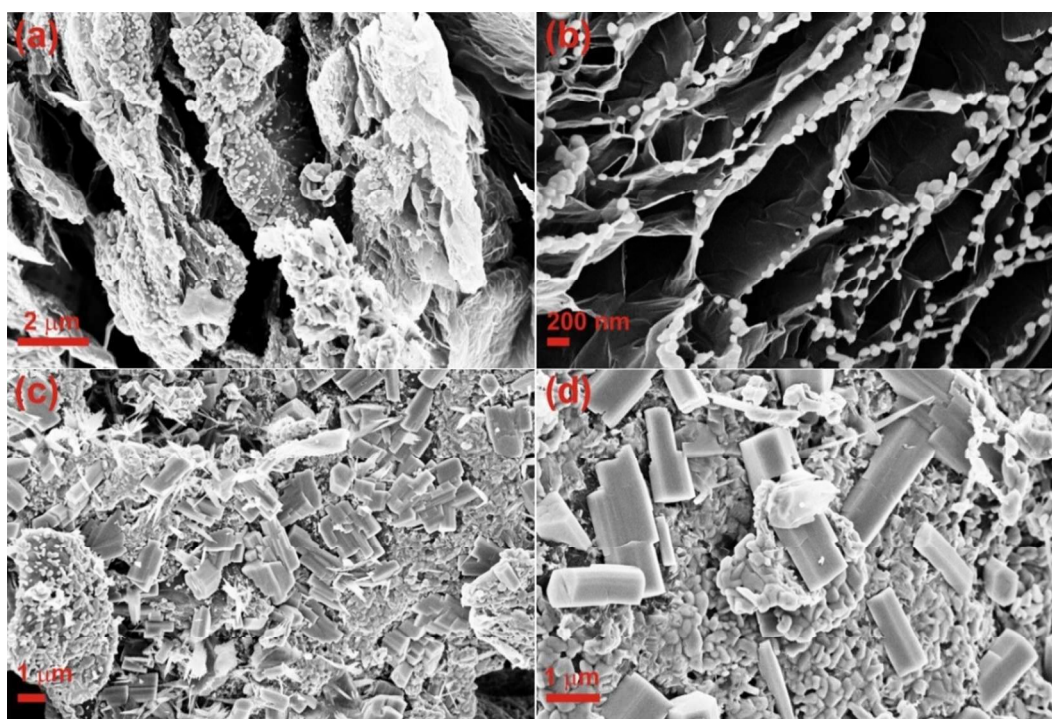**Figure S1.** FESEM images of MoO$_3$ bulk powder at various magnifications.

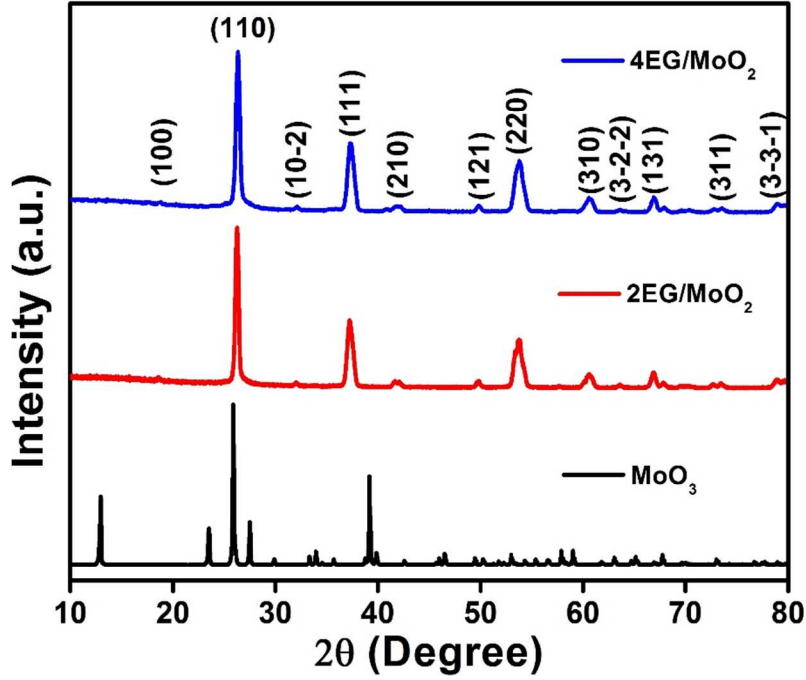**Figure S2.** FESEM images of 2EG/MoO$_2$ at various magnifications.

Figure S3. XRD pattern of 2EG/MoO$_2$ in comparison with those of 2EG/MoO$_2$ and MoO$_3$.

Table S1. Rietveld refinement parameters.

| Structure	2EG/MoO$_2$	4EG/MoO$_2$	MoO$_3$	
	a (Å) = 5.613(3)	a (Å) = 5.620(7)	a (Å) = 3.962(2)	a (Å) = 3.961(5)
Evaluated lattice	b (Å) = 4.860(7)	b (Å) = 4.867(6)	b (Å) = 3.698(3)	b (Å) = 13.852(1)
parameters	c (Å) = 5.627(5)	c (Å) = 5.635(5)	c (Å) = 7.204(6)	c (Å) = 3.695(3)
	β (°) = 120.886	β (°) = 120.879	β (°) = 106.009	--
Crystallite size (Lorentzian)	~42 nm	~33 nm	~222.2 nm	~382.2 nm
Space Group	P2$_1$/c	P2$_1$/c	P2$_1$/m	Pnma
JCPDS file Number	JCPDS # 78-1069	JCPDS # 78-1069	JCPDS # 47-1320	JCPDS # 65-2421
R-Bragg	2.393	1.905	9.391	6.709
Wt% - Rietveld	--	--	96.57	3.43
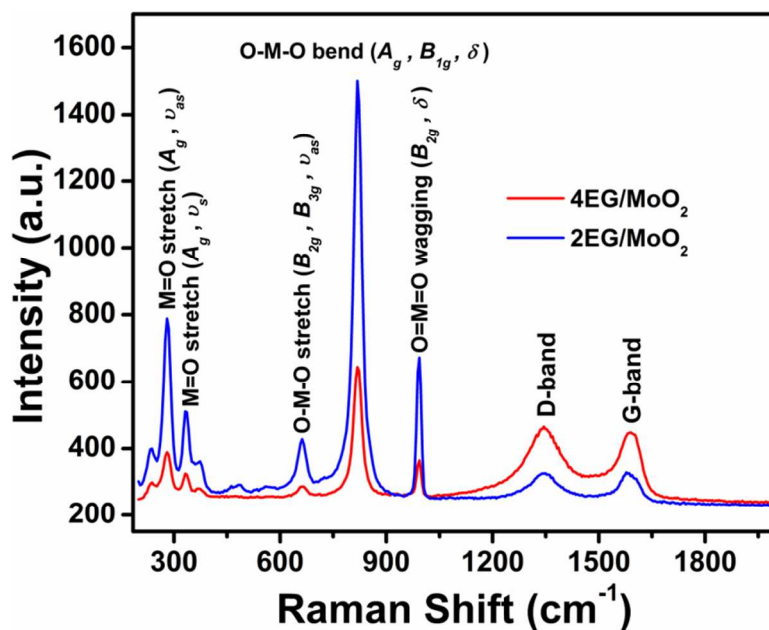
Figure S4. Raman spectra of 2EG/MoO$_2$ and 4EG/MoO$_2$ composites.

Specific surface area measurements

BET and Langmuir surface areas of 2EG/MoO$_2$ are found to be ~3 and ~4 m^2/g respectively. This small specific surface area might be due to the high synthesis temperature, inert nature of the agglomerated MoO$_2$ surfaces and also due to the covering of active surfaces of EG by MoO$_2$. The average pore volume is 0.01 cm^3/g with average pore diameter of ~16 nm. The moderate hysteresis between nitrogen adsorption and desorption isotherms of EG/MoO$_2$ indicates that it possess mesoporosity which might be due to cavities and gaps formed between exfoliated individual graphene layers.

Table S2. BET surface area and porosity details of EG/MoO$_2$ composites.

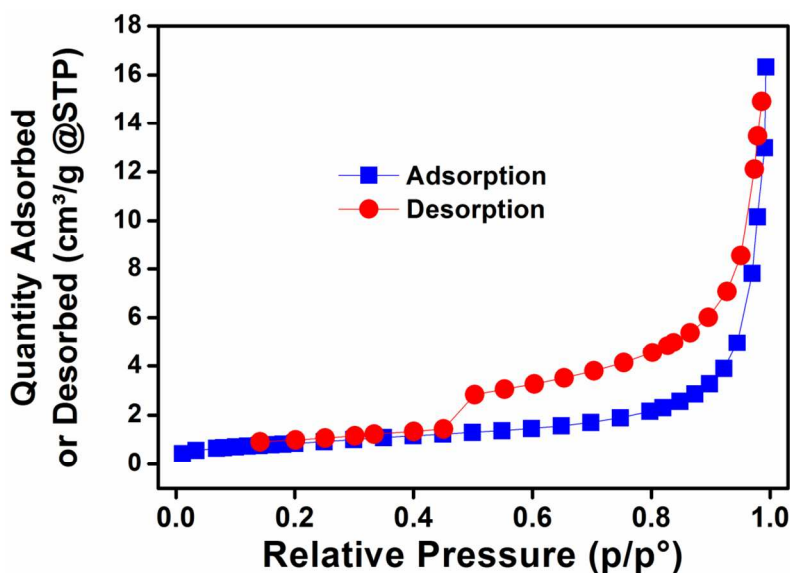| Composite	BET Surface Area	Avg. Pore Size	Avg. Pore Volume
2EG/MoO$_2$	3 m^2/g	~16 nm	0.01 cm^3/g
4EG/MoO$_2$	71 m^2/g	~14 nm	0.24 cm^3/g

Figure S5. BET (N_2) adsorption-desorption isotherms of 2EG/MoO$_2$.

Galvanostatic Intermittent Titration Technique (GITT)

To calculate the diffusion coefficients of cycled 4EG/MoO$_2$, GITT technique was used as follows. A discharge pulse of 50 mA g^{-1} was applied to the battery cycled at 1000 mA g^{-1} to discharge it to a selected voltage and subsequently battery was allowed to rest for 5 h and similar it was done during charging as shown in Fig. S5. Next, the diffusion coefficient for each discharge and charge pulse was calculated by using formula shown in equation S1. The diffusion coefficients of battery cycled at 100 mA g^{-1} are also calculated using above process.

$$D_{Li} = \frac{4}{\pi\tau}\left(\frac{m_B V_m}{M_B A}\right)\left(\frac{\Delta E_S}{\Delta E_\tau}\right)^2 \text{---------- (equation S1)}^1$$

Equation S1 is Li diffusion coefficient formula where

V$_m$ = the molar volume of the compound, **M$_B$** = Formula weight of the active material,

m$_B$ = mass of the active material and **A** = the total contact area between the electrolyte and electrode
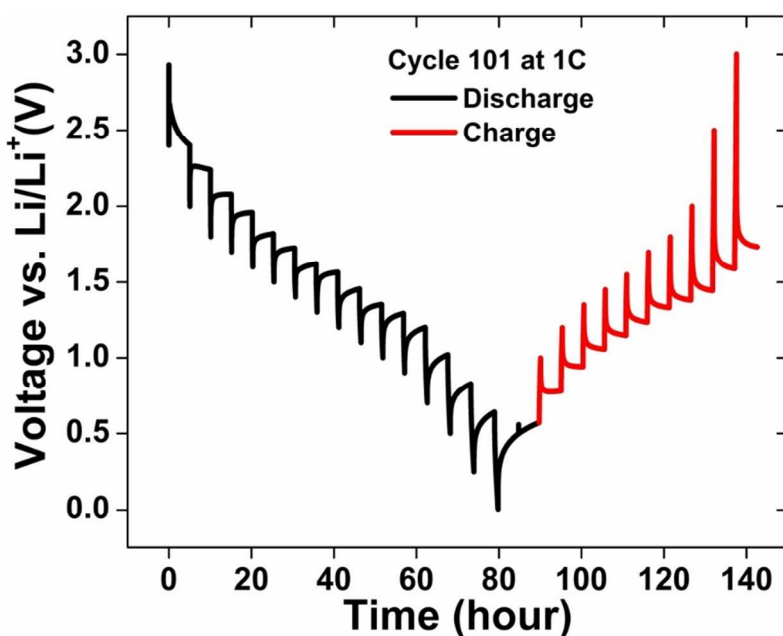
Figure S6. Discharge/charge GITT curves of 4EG/MoO$_2$ cycled at 1000 mA g^{-1}.

Electrochemical impedance spectroscopy results of EG/MoO$_2$ composites

Table S3. Simulated equivalent circuit component values of EG/MoO$_2$ composites.

	R$_e$ (±0.1, Ω)	R$_{ct}$ (±2, Ω)	CPE$_{dl}$ (μF)	C$_i$ (F)
2EG/MoO$_2$@OCV	5.1	98.4	38	0.027
2EG/MoO$_2$@1D	5.6	62.4	41	1.430
2EG/MoO$_2$@1C	5.4	20.6	170	0.029
4EG/MoO$_2$@OCV	4.1	79.32	26.6	0.014
4EG/MoO$_2$@1D	4.5	59.49	38.9	0.640
4EG/MoO$_2$@1C	4.1	14.77	320	0.070

1. Wu, Y.; Reddy, M. V.; Chowdari, B. V. R.; Ramakrishna, S., Long-Term Cycling Studies on Electrospun Carbon Nanofibers as Anode Material for Lithium Ion Batteries. *ACS Applied Materials & Interfaces* **2013,** *5*, 12175-12184.