## **Electronic Supplementary Information for**

Advancing Lithium-Sulfur Battery Efficiency: Utilizing a 2D/2D g-C<sub>3</sub>N<sub>4</sub>@MXene Heterostructure to Enhance Sulfur Evolution Reactions and Regulate Polysulfides in Lean Electrolyte Conditions

Vijay K. Tomer<sup>a,\*</sup>, Otavio Augusto Titton Dias<sup>a</sup>, Abdelaziz M. Gouda<sup>b</sup>, Ritu Malik<sup>a,\*</sup>, Mohini Sain<sup>a,\*</sup>

<sup>a</sup> Department of Mechanical & Industrial Engineering, University of Toronto, Toronto, Canada,
 <sup>b</sup> Solar Fuels Group, Department of Chemistry, University of Toronto, Toronto, Canada

\*Corresponding author: vj.kumar@utoronto.ca; ritu.kumar@utoronto.ca, m.sain@utoronto.ca

Electrode	Condition	R <sub>e</sub>	R <sub>ct</sub>	
g-C <sub>3</sub> N <sub>4</sub> -Mx/S	Fresh cell	4.0	34.9	
	After 190 cycles	4.9	30.1	
g-C <sub>3</sub> N <sub>4</sub> /S	Fresh cell	8.1	58.3	
	After 105 cycles	8.6	45.7	

**Table S1:** Results obtained from Nyquist plot for fresh and cycled cells.

**Table S2:** Comparison of Li-S battery performance with previously published works.

Host material	Specific surface	Sulfur	Initial	Retained	Rate	Cycle	Capacity	Ref
	area (m²/g)	content	capacity	capacity		number	retention (%) =	
		(%)	(mAh/g) <sup>a</sup>	$(\mathbf{mAh/g})^{\mathbf{b}}$			<u>b</u>	
							a x 100	
g-C <sub>3</sub> N <sub>4</sub> nanosheets	209	70.4	870	578	0.5 C	750	66.43	1
g-C <sub>3</sub> N <sub>4</sub> spheres	931	69.8	934	775	0.5 C	100	82.97	2
Porous g-C <sub>3</sub> N <sub>4</sub>	83	68.67	734	620	1 C	300	84.46	3
g-C <sub>3</sub> N <sub>4</sub> /C porous cages	428	67	1240	729	1 C	200	58.79	4
Hierarchically porous g-	498	64.5	1150	1128	0.2 C	100	98.08	5
$C_3N_4/C$								
3D porous g-C <sub>3</sub> N <sub>4</sub> /	827	731	1132	974	0.2 C	800	86.04	6
graphene sponge								
3D porous g-C <sub>3</sub> N <sub>4</sub> / CNT	202	80	1023	583	1 C	500	56.98	7
3D g-C <sub>3</sub> N <sub>4</sub> /rGO/CNT	225	70.8	730	620	1 C	500	84.93	8
microspheres								
g-CN + MXene	54	69.5	1061	73	C/8	190	73	This
								work



Figure S1: Zeta potential value of pure g-C<sub>3</sub>N<sub>4</sub> nanosheets and MXene nanosheets.



Figure S1: N<sub>2</sub> sorption isotherms for the as-prepared materials.



Figure S3: TGA profile of sulfur-based composite.



**Figure S4:** XPS survey scan for g-C<sub>3</sub>N<sub>4</sub>-Mx/S composite.



Figure S5: Cycle performance of the g- $C_3N_4$ -Mx/S cathode with varied sulfur loading for 190 cycles at C/8.



Figure S6: EIS spectra of  $g-C_3N_4$ -Mx/S cathode extracted from the pouch cell after 190 charge-discharge cycles.



**Figure S7:** Complete XPS scan spectrum of the  $g-C_3N_4$ -Mx/S cathode obtained from the pouch cell cycled for 190 charge-discharge cycles.

## **References:**

- 1 Z. Meng, Y. Xie, T. Cai, Z. Sun, K. Jiang and W. Q. Han, *Electrochimica Acta*, 2016, **210**, 829–836.
- Z. Meng, S. Li, H. Ying, X. Xu, X. Zhu and W. Q. Han, *Advanced Materials Interfaces*, 2017, 4, 1601195.
- 3 D. Li, J. Liu, W. Wang, S. Li, G. Yang, P. Wang, K. Zhu and Z. Li, *Applied Surface Science*, 2021, **569**, 151058.
- 4 P. Song, Z. Chen, Y. Chen, Q. Ma, X. Xia and H. Liu, *Electrochimica Acta*, 2020, **363**, 137217.
- 5 X. Hong, Y. Liu, J. Fu, X. Wang, T. Zhang, S. Wang, F. Hou and J. Liang, *Carbon*, 2020, **170**, 119– 126.
- 6 J. Zhang, J. Y. Li, W. P. Wang, X. H. Zhang, X. H. Tan, W. G. Chu and Y. G. Guo, *Advanced Energy Materials*, 2018, **8**, 1702839.
- 7 W. He, X. He, M. Du, S. Bie, J. Liu, Y. Wang, M. Liu, Z. Zou, W. Yan and H. Zhao, *Journal of Physical Chemistry C*, 2019, **123**, 15924–15934.
- J. Wang, Z. Meng, W. Yang, X. Yan, R. Guo and W. Q. Han, *ACS Applied Materials and Interfaces*, 2019, **11**, 819–827.