Electronic Supplementary information

Silicon Nanoparticles Sandwiched Ultrathin MoS_2-Graphene Layers as an Anode Material for Li-Ion Battery

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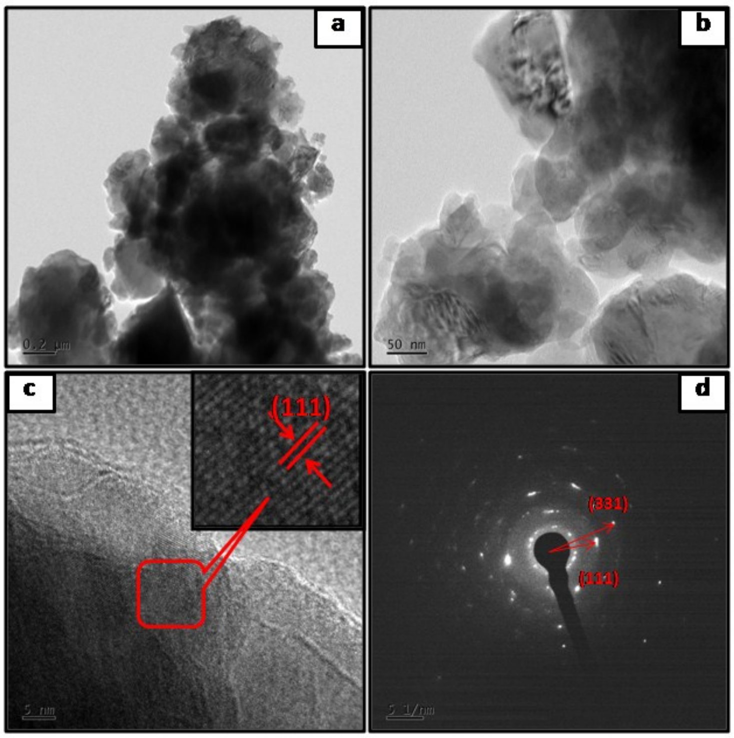

Fig.S1 TEM of Silicon (a,b) at different magnifications ; (c) HRTEM of the Silicon ; (d)corresponding SAED pattern

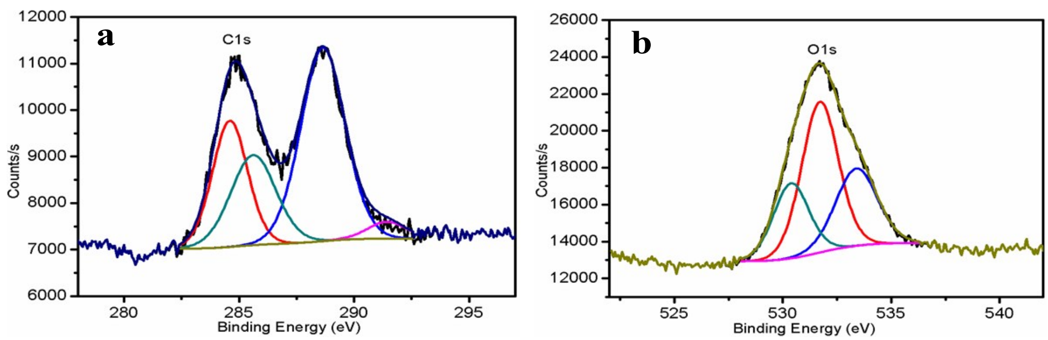

Fig.S2 XPS spectra of the Si@MoS_2-G(1:2-S2) for (a) C1s and (b) O.

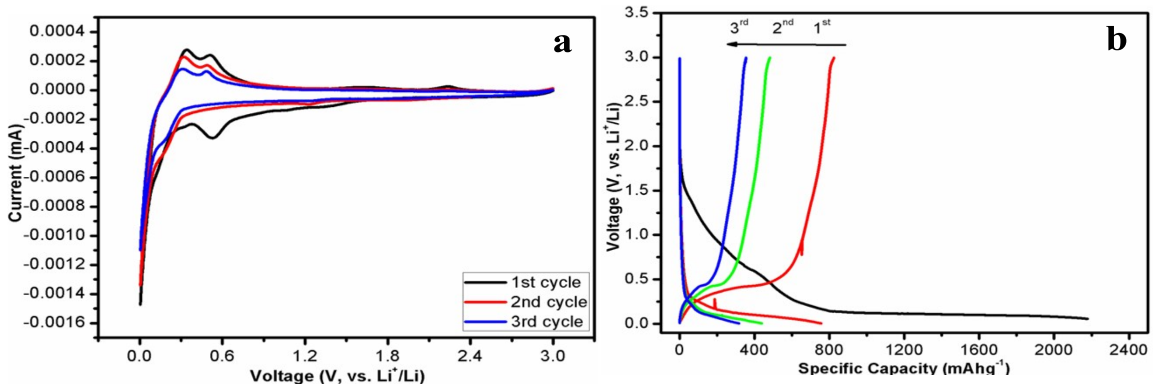

Fig.S3(a) Cyclic voltametry at a scan rate of 0.1 mV s^{-1} (b) the initial discharge-charge profiles of Si@MoS$_2$-G (2:1-S3)

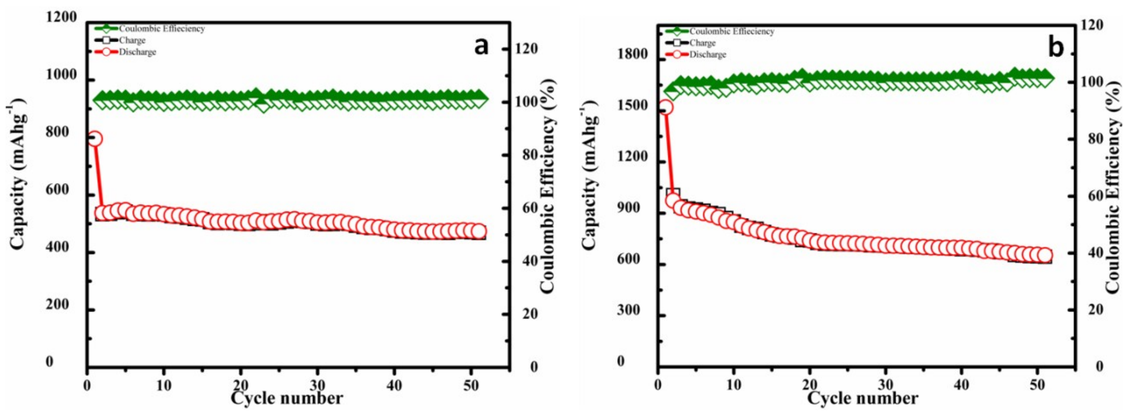

Fig.S4 cycling performance of Si- MoS$_2$ between 0.01 and3V at the current density of 1000 mAg^{-1} of (a)MoS$_2$-G (S1), (b) Si@MoS$_2$-G (1:2-S2)

Figure S5 and S6 shows the FESEM-EDS spectrum of S1, S2 and S3 electrode material before and after cycling which clearly indicates the existence of silicon, molybdenum and sulfur contents in respective samples. Respective results tabulated in Table S1 and S2. Under close examination, the Si@MoS$_2$-G (S3) having more cracks compared to the Si@MoS$_2$-G (S2) shown in figure S7. It reveals that the MoS$_2$-G layers unable to prevent volume change at higher concentration of Si. It suggests better stability characteristics with the Si@MoS$_2$-G (S2) compared to the Si@MoS$_2$-G (S3).

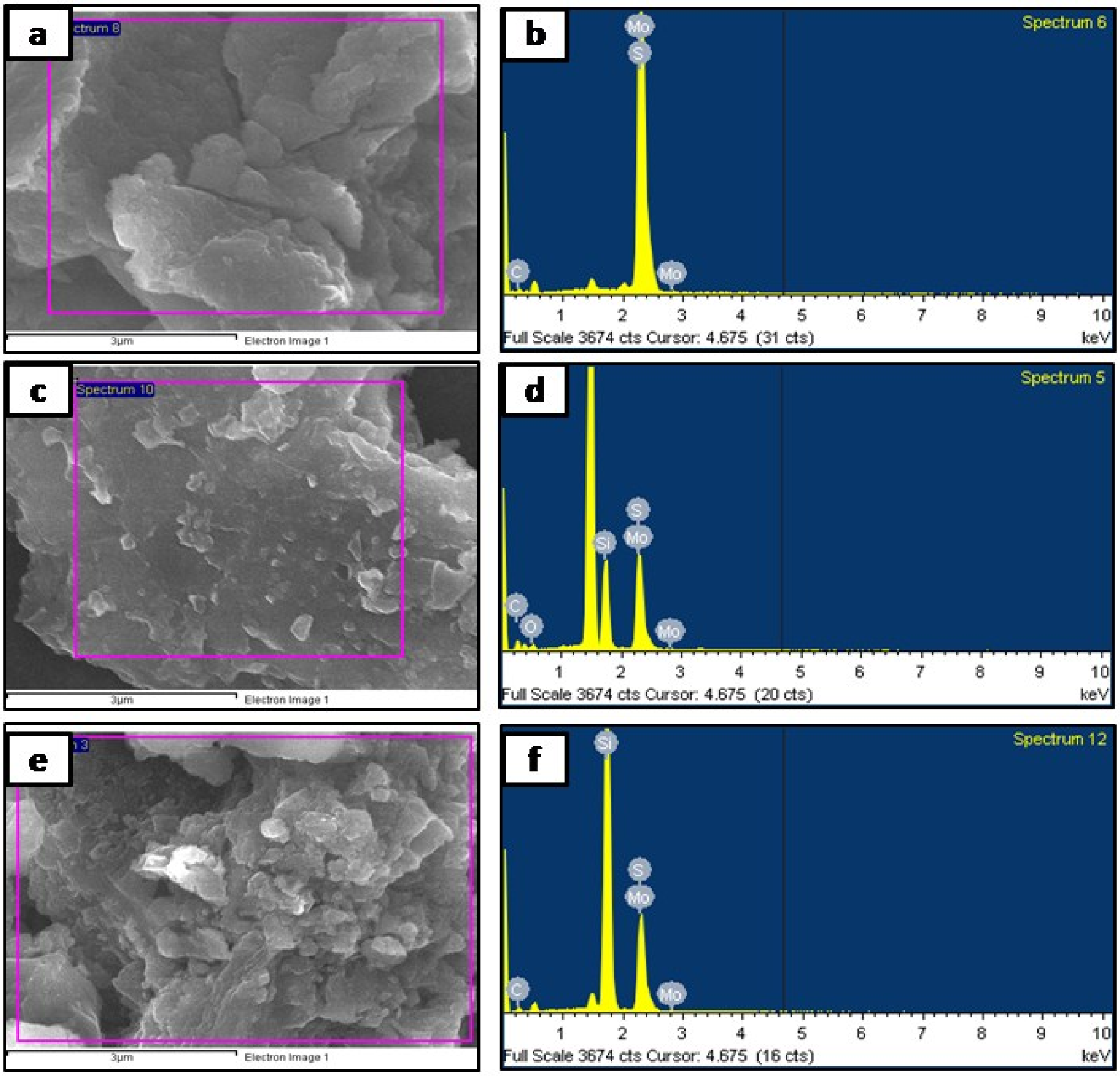

Fig.S5. FESEM-EDS spectrum of S1, S2 and S3 samples

Table S1: Elements analyzed of sample S1, S2 and S3 before cycling via FESEM-EDS

	S1		S2		S3	
Element	Weight %	Atomic %	Weight %	Atomic %	Weight %	Atomic %
C K	25.48	60.34	27.67	54.91	25.38	49.9
Si K	-	-	31.72	26.92	43.28	36.4
S K	29.75	26.39	16.33	12.14	12.2	8.98
Mo L	44.77	13.27	24.28	6.03	19.15	4.71
Totals	100		100		100	

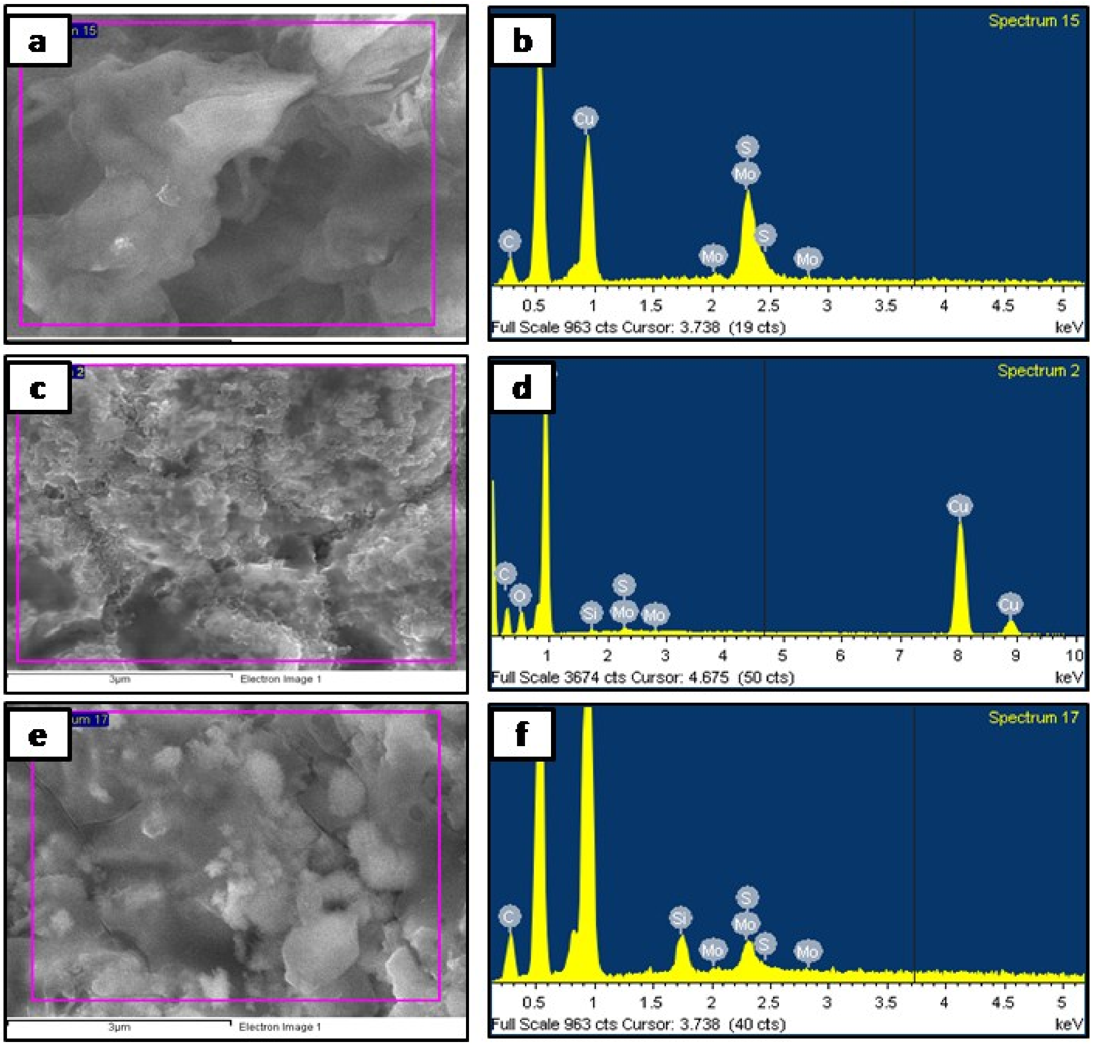

Fig.S6. FESEM-EDS spectrum of S1, S2 and S3 samples after cycling

Table S2: Elements analyzed of sample S1, S2 and S3 after cycling via FESEM-EDS

	S1		S2		S3	
Element	Weight %	Atomic %	Weight %	Atomic %	Weight %	Atomic %
C K	31.10	71.08	35.98	73.51	63.09	83.85
Si K	-	-	2.76	2.41	19.93	11.33
S K	3.04	2.61	3.50	2.68	3.35	1.67
Mo L	14.66	4.20	6.93	1.77	3.17	0.53
Cu	51.20	22.12	50.83	19.63	10.46	2.63
Totals	100		100		100	

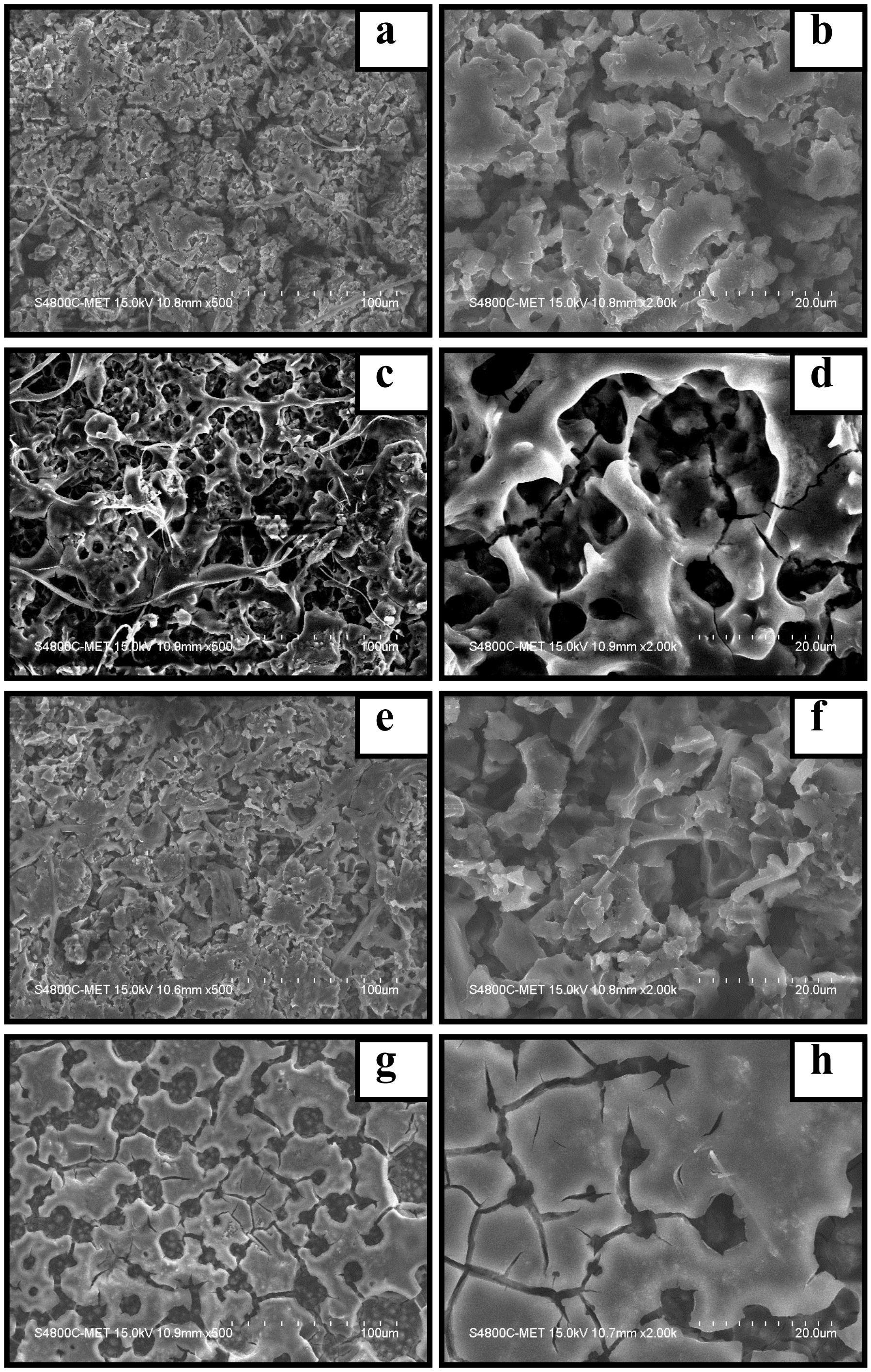

Fig.S7. FESEM images obtained from the cycled Pure Si (a, b); MoS_2-G (c, d) Si@MoS_2-G (S1) (e, f) and Si@MoS_2-G(S3) (g, h) composite electrodes.

Table S3. Comparison of the electrochemical properties composites of Silicon/MoS_2 with other structures

No	Current density (mAg^{-1})	Capacity $mAhg^{-1}$ (at initial Cycle)	Rate performance capacity (mAh g-1) @ current density(mA g−1) (cycle)	Reference
1	50	861	710 @200 (100)	Si/C yolk/shell[1]
2	300	2286	880 @51 (300)	Si@lignocellulose [2]
3	60	~800	-	Si-SiC-Ni[3]
4	100	1296	940 @100 (200)	$FeSi_2$/Si@C[4]
5	100	800	~1000(10)	Si/graphite[5]
6	200	832	652@200 (100)	Si /graphite/carbon[6]
7	100	470	554@100 (50)	Hollow Si/C[7]
8	35	840–994	400–509@70 (100)	silicon oxycarbide fiber[8]
9	200	1083.5	~630@1600(400)	MoS_2/CFs[9]
10	50	1200	1080 @800 (200)	MoS_2 / SnO_2[10]
11	200	1002	989.7 @ 200 (60)	MoS_2/SnS[11]
12	50	871	802 @100 (50)	MoS_2/TiO_2[12]
13	100	979	660@1000 (50)	SnO_2/MoS_2[13]
14	100	623.5	417@100 (20)	SiCN-MoS_2[14]
15	20	799	677@200(90)	Present work (MoS_2-G)
16	20	1549	923@200(90)	present work (Si@MoS_2-G)

Notes and references

1. X. Huang, X. Sui, H. Yang, R. Ren, Y. Wu, X. Guo and J. Chen, *Journal of Materials Chemistry A*, 2018, DOI: 10.1039/C7TA08283E.
2. C.-Y. Chou, J.-R. Kuo and S.-C. Yen, *ACS Sustainable Chemistry & Engineering*, 2018, **6**, 4759-4766.
3. T.-Y. Huang, B. Selvaraj, H.-Y. Lin, H.-S. Sheu, Y.-F. Song, C.-C. Wang, B. J. Hwang and N.-L. Wu, *ACS Sustainable Chemistry & Engineering*, 2016, **4**, 5769-5775.
4. Y. Chen, J. Qian, Y. Cao, H. Yang and X. Ai, ACS Appl. Mater. Interfaces, 2012, **4** , 3753–3758 .
5. T. Mochizuki, S. Aoki, T. Horiba, M. Schulz-Dobrick, Z.-J. Han, S. Fukuyama, H. Oji, S. Yasuno and S. Komaba, *ACS Sustainable Chemistry & Engineering*, 2017, **5**, 6343-6355.
6. W. Liu, Y. Zhong, S. Yang, S. Zhang, X. Yu, H. Wang, Q. Li, J. Li, X. Cai and Y. Fang, *Sustainable Energy & Fuels*, 2018, DOI: 10.1039/C7SE00542C.
7. H. Zhang, X. Li, H. Guo, Z. Wang and Y. Zhou, *Powder Technology*, 2016, **299**, 178-184.
8. A. Tolosa, M. Widmaier , B. Kruner, J. M. Griffin and V. Presser, *Sustainable Energy & Fuels*, 2018, **2**, 215-228.
9. D. Ren, Y. Hu, H. Jiang, Z. Deng, S. Petr, H. Jiang and C. Li, *ACS Sustainable Chemistry & Engineering*, 2016, **4**, 1148-1153.
10. M. Li, Q. Deng, J. Wang, K. Jiang, Z. Hu and J. Chu, *Nanoscale*, 2018, **10**, 741-751.
11. Q. Pan, F. Zheng, Y. Wu, X. Ou, C. Yang, X. Xiong and M. Liu, *Journal of Materials Chemistry A*, 2018, **6**, 592-598.

12. X. Zhu, X. Liang, X. Fan and X. Su, *RSC Advances*, 2017, **7**, 38119-38124.
13. J. L. Y. Chen, W. and L. L. a. J. X. Shi, , , *J. Mater. Chem. A*, 2014, DOI: DOI: 10.1039/C4TA03770G.
14. L. David, R. Bhandavat, U. Barrera and G. Singh, *Scientific Reports*, 2015, **5**, 9792.