

Supplementary Information

Insight into the Storage Mechanism of Sandwich-Like Molybdenum Disulphide/Carbon Nanofibers Composite in Aluminum-Ion Batteries

Xiaobing Wang ¹, Ruiyuan Zhuang ^{2,*}, Xinyi Liu ¹, Mingxuan Hu ¹, Panfeng Shen ¹, Jintao Luo ¹, Jianhong Yang ³ and Jianchun Wu ^{3,4,*}

¹ School of Advanced Materials Engineering, Jiaxing Nanhu University, Jiaxing 314000, China; 202145575121@jxnhu.edu.cn (X.W.); 202145675122@jxnhu.edu.cn (X.L.); 202145895115@jxnhu.edu.cn (M.H.); 202145905121@jxnhu.edu.cn (P.S.); 202145905123@jxnhu.edu.cn (J.L.)

² School of Mechanical and Electrical Engineering, Jiaxing Nanhu University, Jiaxing 314000, China

³ School of Materials Science and Engineering, Jiangsu University, Zhenjiang 212013, China; jhyang@ujs.edu.cn

⁴ Institute of Nuclear Science and Technology, Sichuan University, Chengdu 610064, China

* Correspondence: zhuangryuan@jxnhu.edu.cn (R.Z.); jcwu@ujs.edu.cn (J.W.)

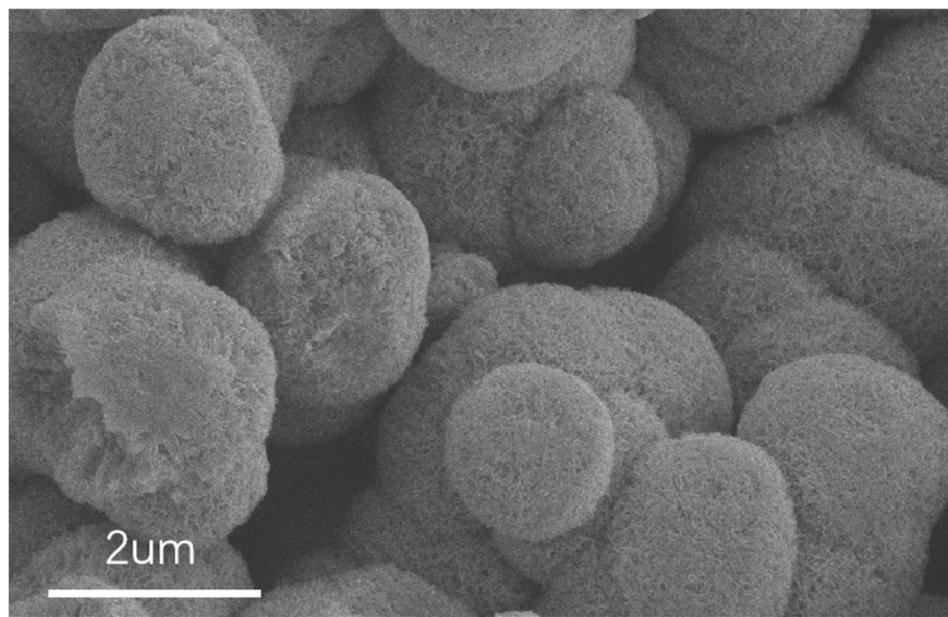


Figure S1 Scanning electron microscopy (SEM) images of MoS_2 .

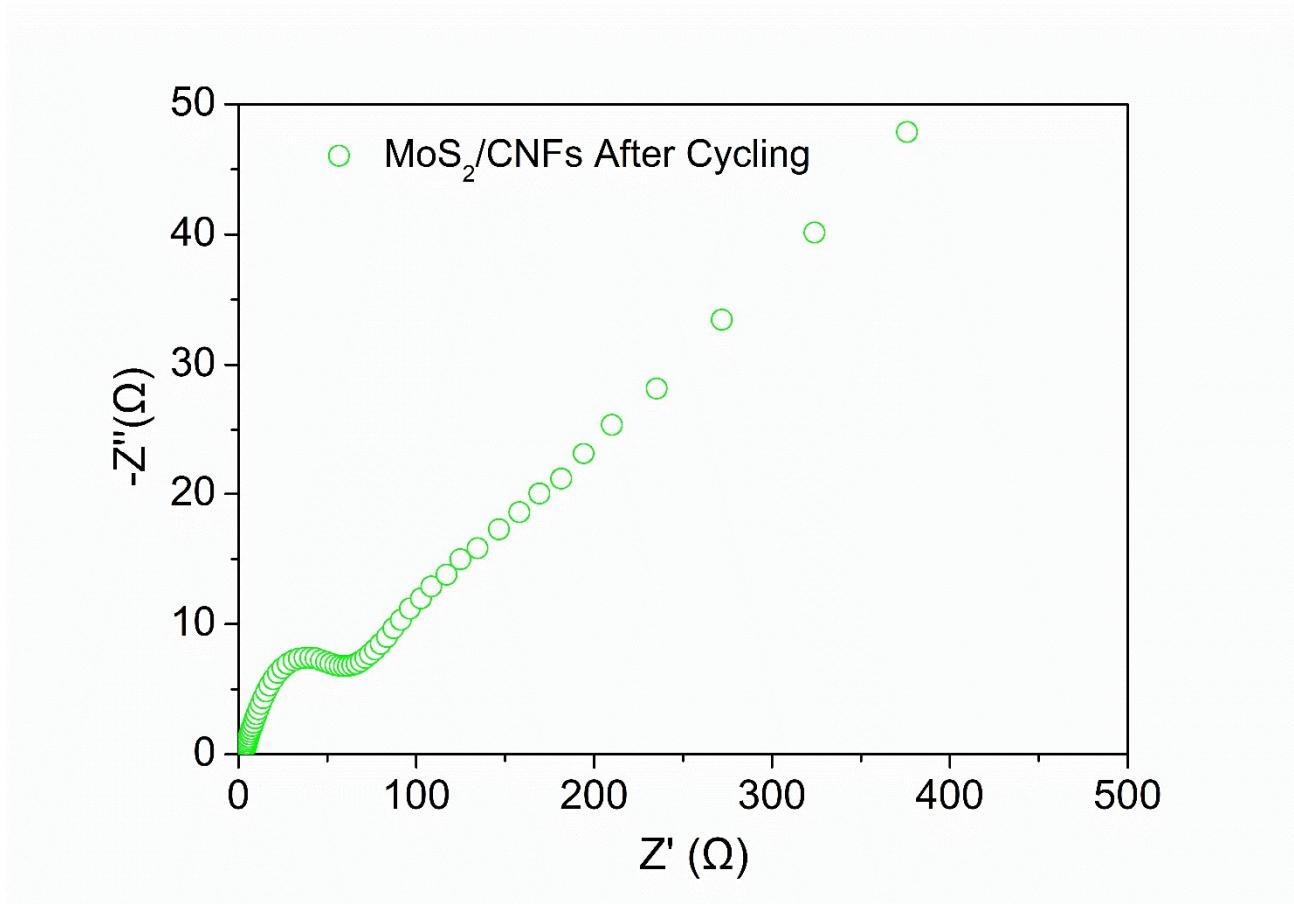


Figure S2 Nyquist plots of MoS_2/CNFs after cycling.

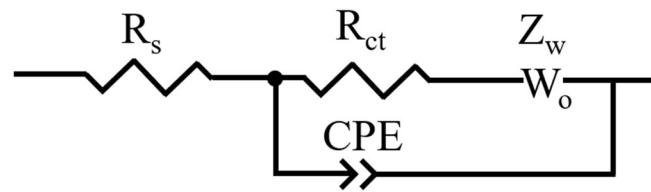


Figure S3 Equivalent circuit model.

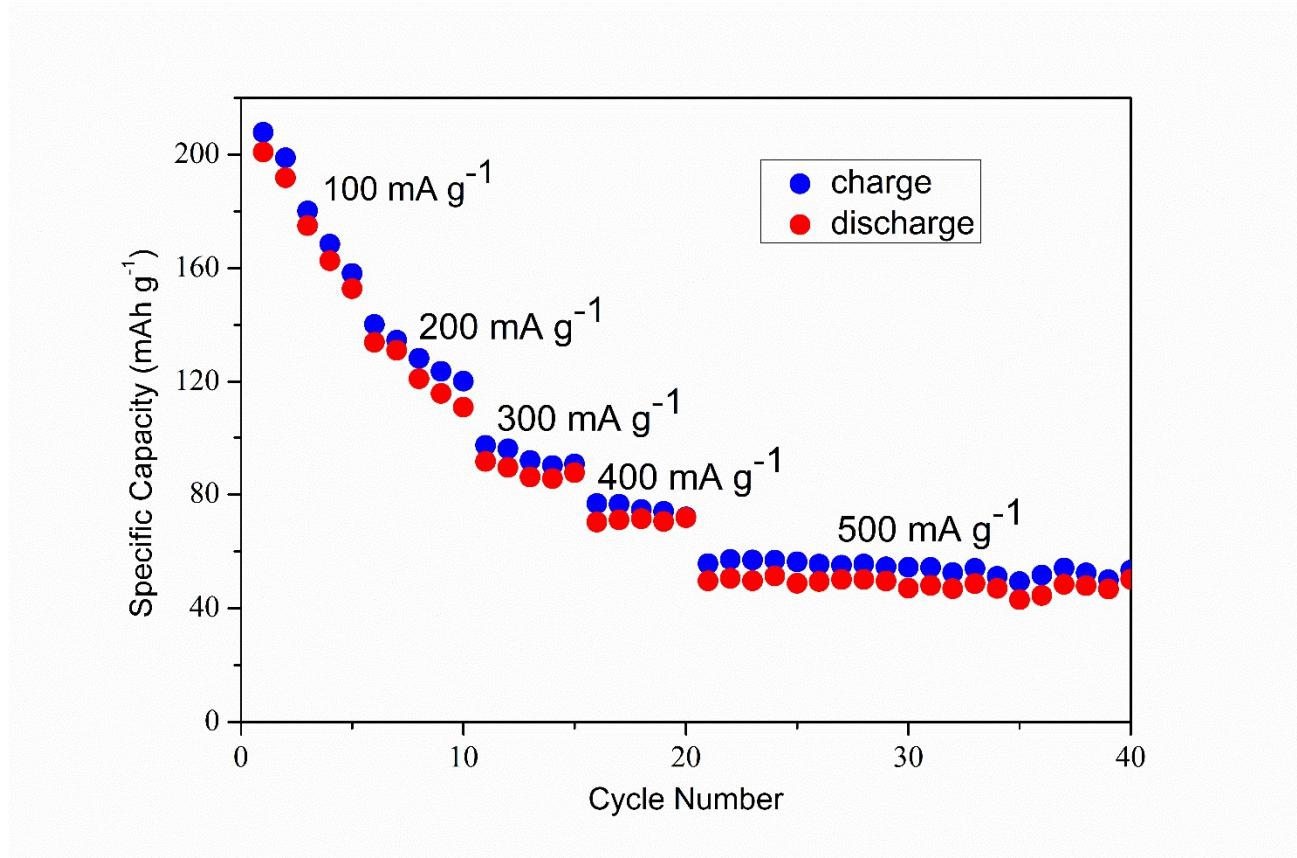


Figure S4 Rate performance of MoS₂/CNFs electrode at different current density.

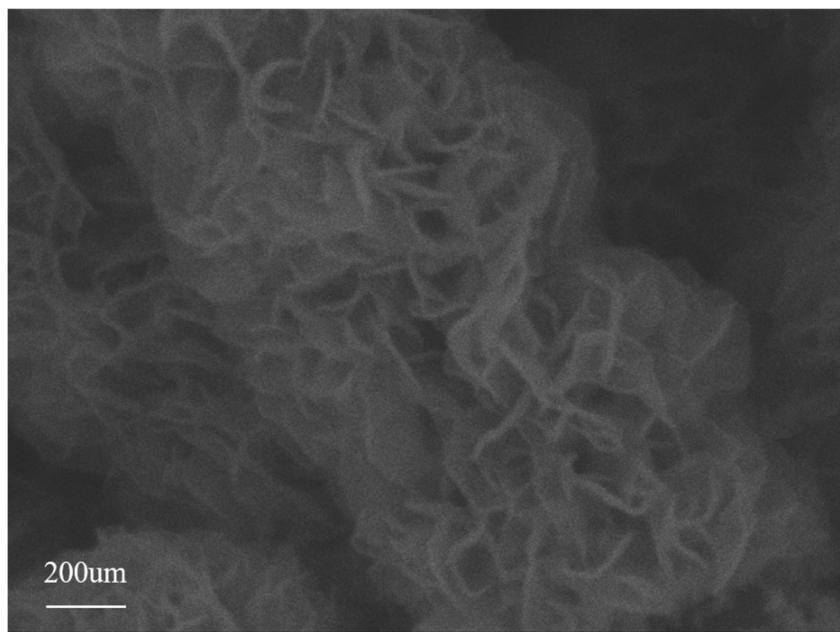


Figure S5 Scanning electron microscopy (SEM) images of MoS₂/CNFs after cycling.

Table S1 Performance comparison of MoS₂/CNFs with several other transition metal dichalcogenides for application in AIBs

Cathode materials	Cycle number	Current density (mA g ⁻¹)	Specific capacity (mAh g ⁻¹)	Ref.
Graphene-VS ₂	50	100	50	[39]
	120	400	129.24	[40]
	100	100	60	[41]
	50	12	70	[42]
	150	50	90	[43]
	100	200	70	[44]
	50	5	85	[45]
	100	300	80	[46]
	100	100	198	[47]
	500	1000	119	[48]
	100	200	70	[49]
	100	40	66.7	[27]
CoS ₂ /CNT	100	100	60	[50]
MoS₂/CNFs	200	100	66	This work

Table S2 The formation energy of aluminum ions embedded in different channels of MoS₂

the possible entry pathways for aluminum ions	Total energy (eV)	Formation energy (eV)
Channel 1	-716.86	5.34
Channel 2	-720.62	0.64