Electronic Supplementary Material (ESI) for Green Chemistry.

Supplemental Materials

Multi-stage explosion of lignin: A new horizon for constructing defect-rich carbon towards advanced lithium ion storage

Caiwei Wang[a], Dongjie Yang[a,*], Si Huang[a], Yanlin Qin[b,c], Wenli Zhang[b,c] and Xueqing Qiu[b,c,*]

[a] *School of Chemistry and Chemical Engineering, Guangdong Provincial Engineering Research Center for Green Fine Chemicals, South China University of Technology, Guangzhou 510640, China*

[b] *School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou, 510006, China*

[c] *Guangdong Provincial Key Laboratory of Plant Resources Biorefinery, 100 Waihuan Xi Road, Panyu District, Guangzhou 510006, China*

***Corresponding Authors:** Prof. Dongjie Yang, Xueqing Qiu

***E-mail address*:** cedjyang@scut.edu.cn (D. Yang), cexqqiu@scut.edu.cn (X. Qiu).

Table of Contents

Supplementary Figures

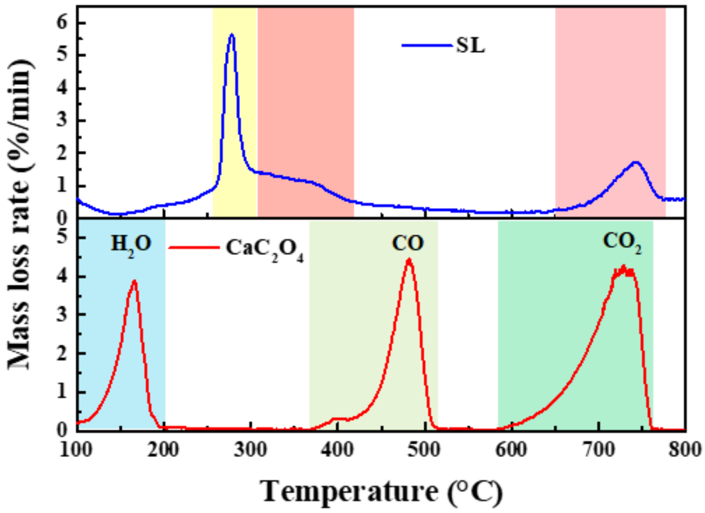

Fig. S1. DTG curves of SL and CaC_2O_4.

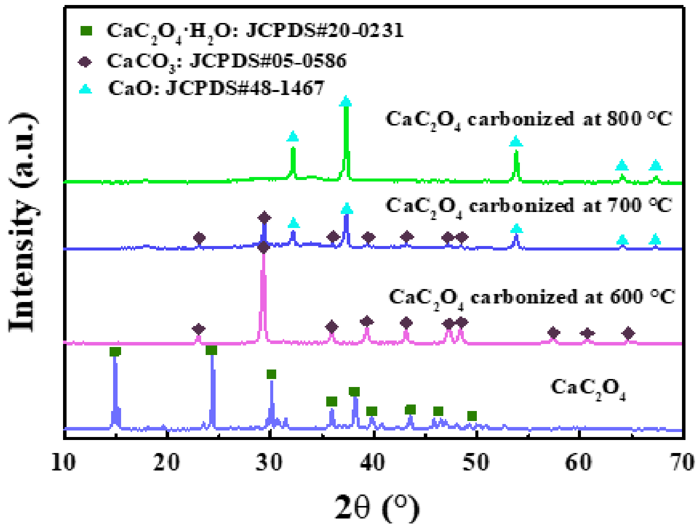

Fig. S2. XRD patterns of CaC_2O_4 carbonized at 600-800 °C. The diffraction peak of pure CaC_2O_4 fits well with that of $CaC_2O_4 \cdot H_2O$ (JCPDS #20-0231). The diffraction peak of CaC_2O_4 carbonized at 600 °C accords well with those of $CaCO_3$ (JCPDS #05-0586), indicating that CaC_2O_4 was completely decomposed into $CaCO_3$ at 600 °C. CaC_2O_4 carbonized at 700 °C presents the diffraction peak in good agreement with $CaCO_3$ (JCPDS #05-0586) and CaO (JCPDS #48-1467), indicating that $CaCO_3$ was partially decomposed into CaO at 700 °C. The diffraction peak of CaC_2O_4 carbonized at 800 °C coincides with those of CaO (JCPDS 48-1467), indicating $CaCO_3$ was completely decomposed into CaO at 800 °C.

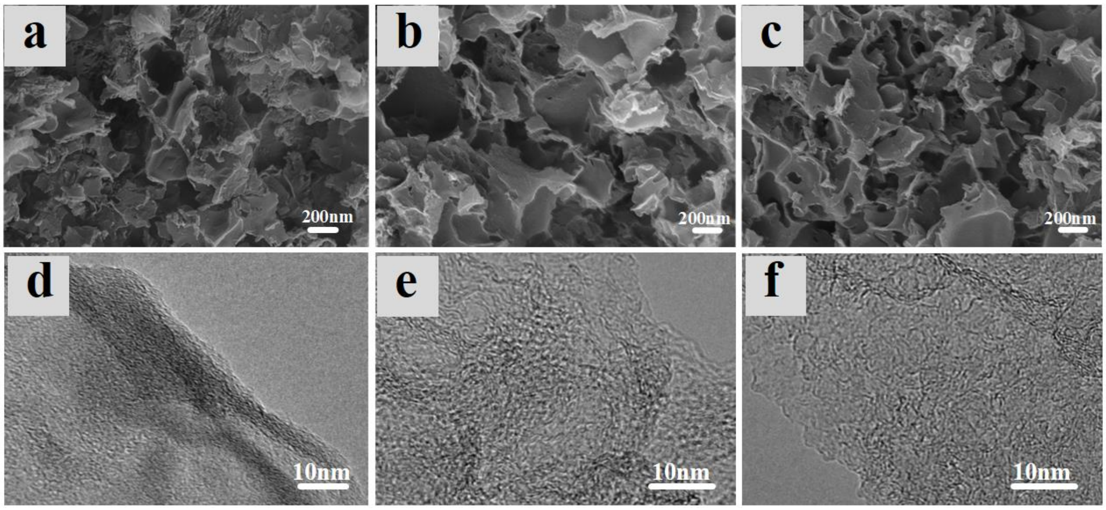

Fig. S3. SEM images of (a) PLPCC-600, (b) PLPCC-700, (c) PLPCC-800. HRTEM images of (d) PLPCC-600, (e) PLPCC-700, (f) PLPCC-800.

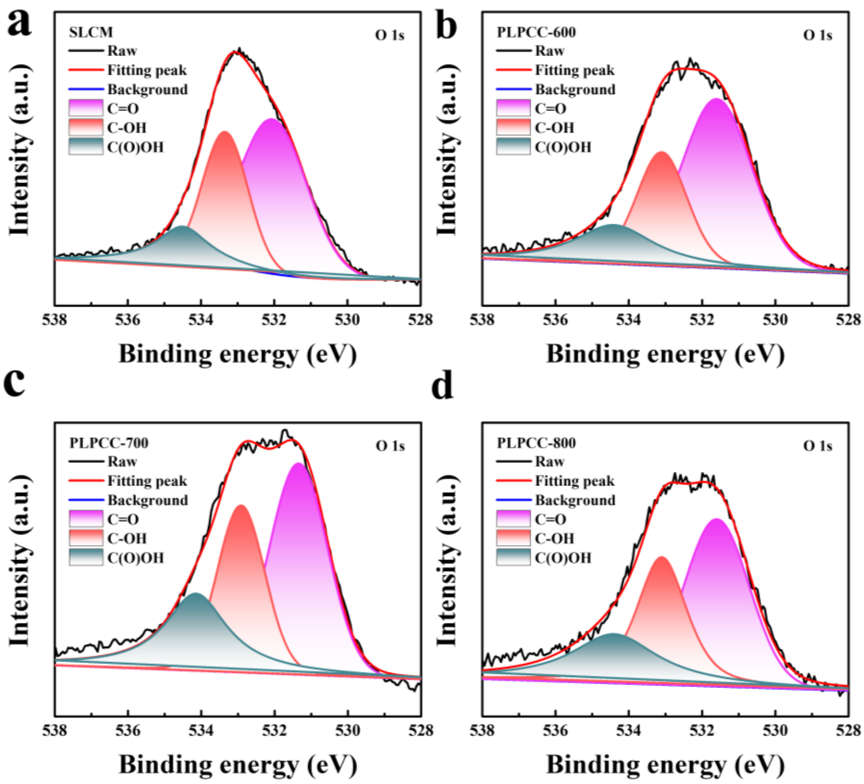

Fig. S4. Deconvolution of high-resolution O 1s spectra of PLPCCs and SLCM.

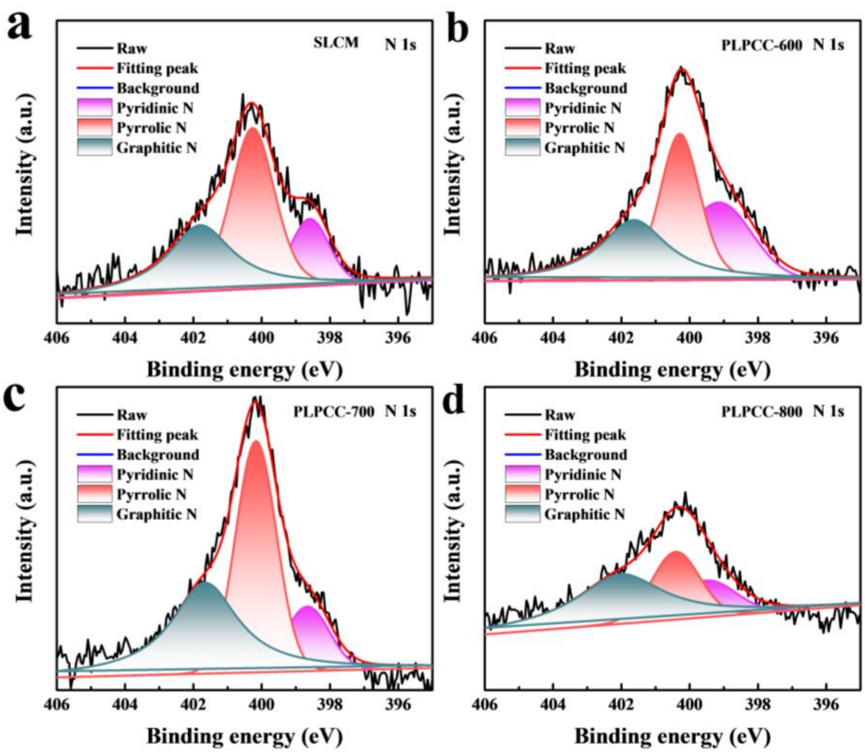

Fig. S5. Deconvolution of high-resolution N 1s spectra of PLPCCs and SLCM.

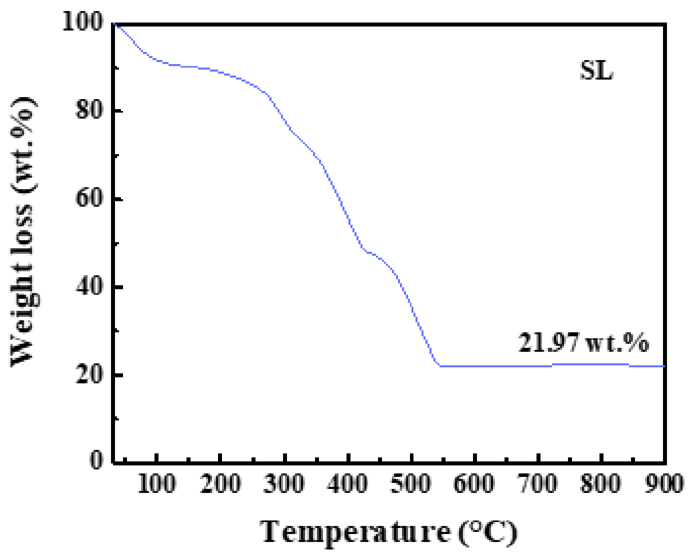

Fig. S6. TG curves of SL under air atmosphere. After air heat treatment at 900 °C, the ash residue of SL is 21.97 wt.%.

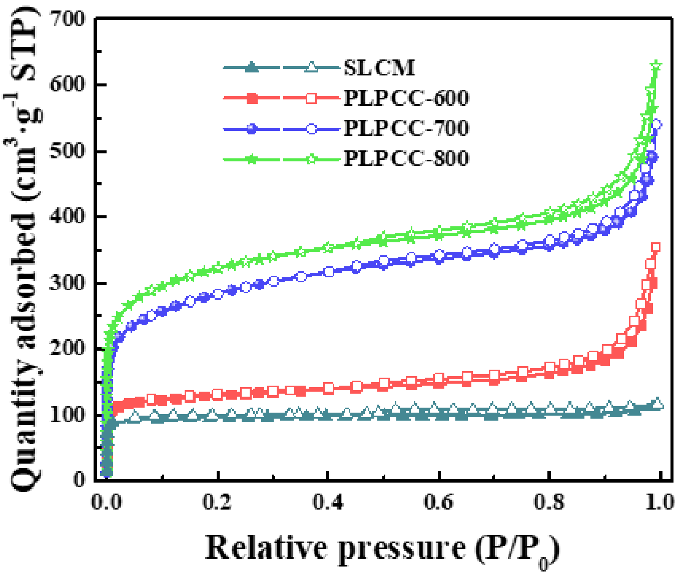

Fig. S7. Nitrogen adsorption and desorption isotherms.

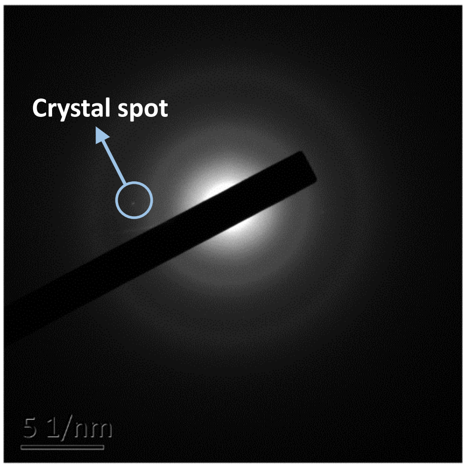

Fig. S8. SEAD pattern of PLPCC-700.

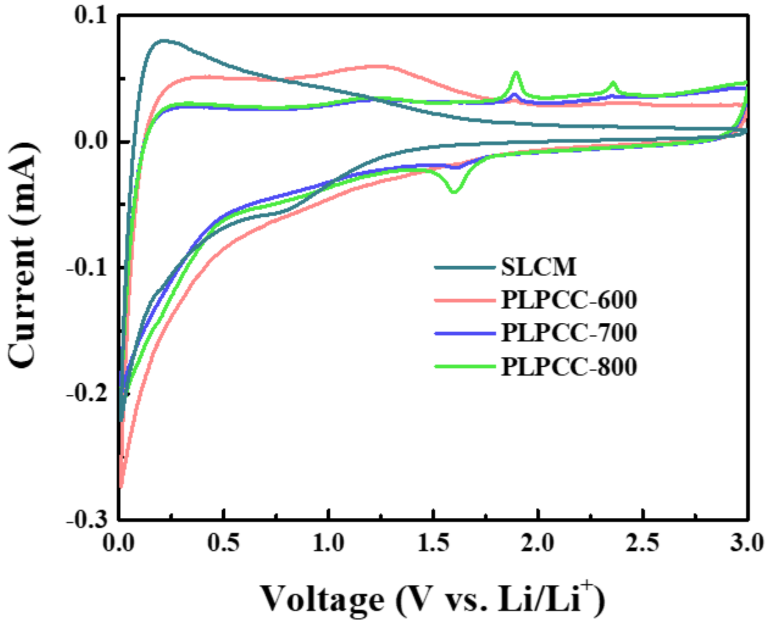

Fig. S9. The first CV curves of electrodes.

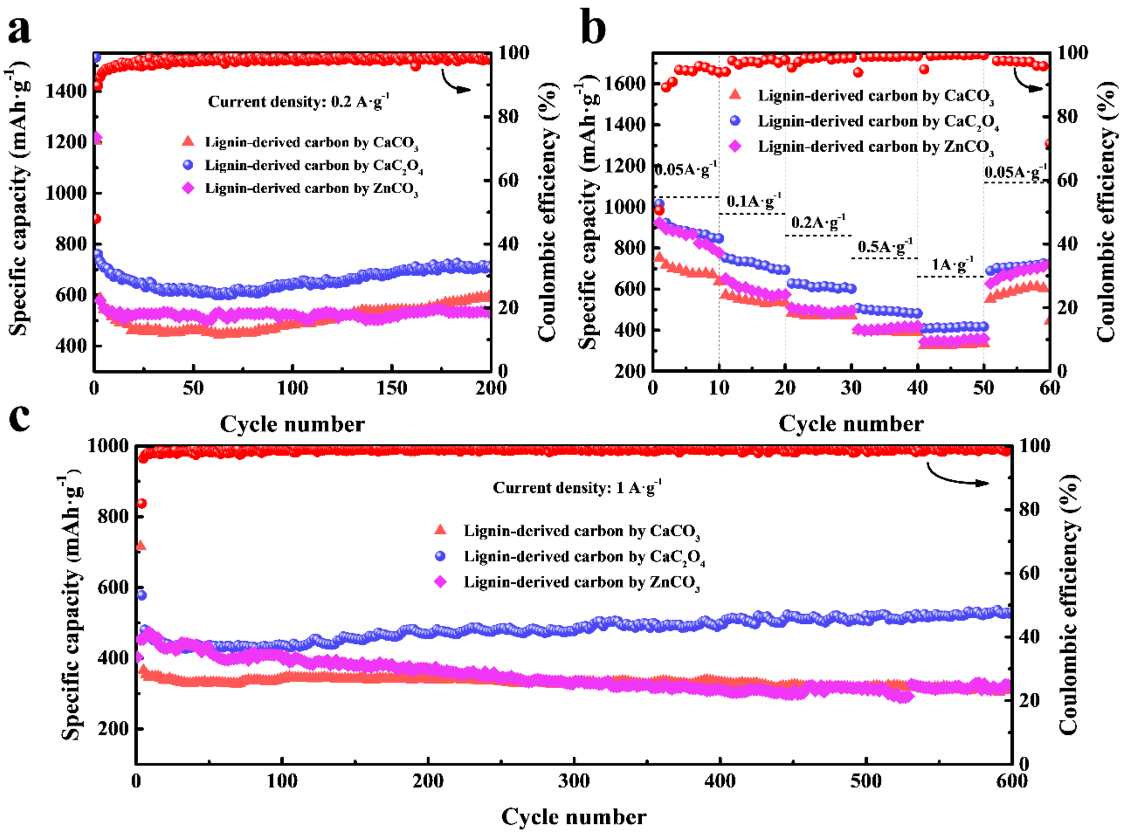

Fig. S10. Comparison of lithium storage capabilities of the lignin-derived carbons prepared by $CaCO_3$, CaC_2O_4 and $ZnCO_3$. (a) GCD curves at 0.2 A·g^{-1}. (b) Rate performance at 0.05-1 A·g^{-1}. (c) Long-cycling performance at 1 A·g^{-1}.

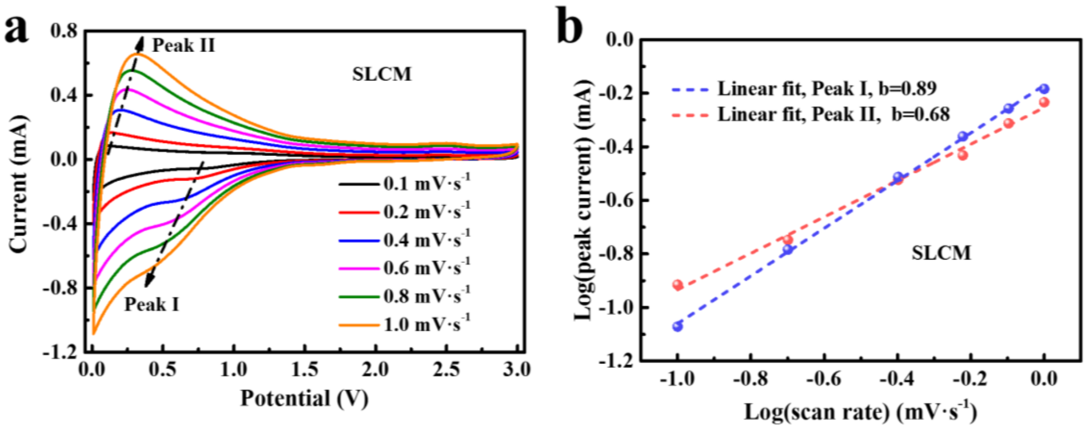

Fig. S11. (a) CV curves of SLCM at different scan rates. (b) Determination of *b* values.

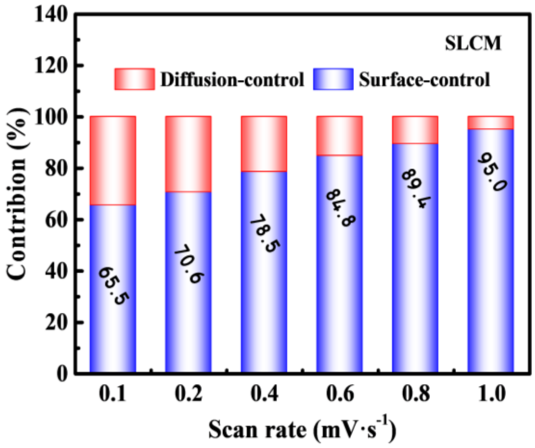

Fig. S12. (a) Capacitance-controlled and diffusion-controlled contribution of SLCM.

Supplementary Tables

Table S1 Surface O and N configurations of SLCM and PLPCCs.

Samples	Percentage of *O*-containing groups			Percentage of *N*-containing groups		
	C=O	C-OH	COOH	N-6	N-5	N-Q
SLCM	28.2	47.2	24.6	15.9	46.2	37.9
PLPCC-600	53.3	27.3	19.4	24.5	37.0	38.5
PLPCC-700	52.3	25.0	22.7	13.2	43.9	42.8
PLPCC-800	43.2	31.5	25.3	17.7	27.6	54.7

Table S2 Textural properties of SLCM and the PLPCC samples at 600-800°C.

Samples	S_{BET} (m^2/g)	V_{total} (cm^3/g)	V_{mic} (cm^3/g)	V_{meso} (cm^3/g)	V_{mic}/V_{total} (%)	V_{meso}/V_{total} (%)	D_{avg} (nm)
SLCM	385.5	0.15	0.12	0.02	80.0	13.3	1.87
PLPCC-600	491.3	0.49	0.17	0.23	34.7	46.9	3.01
PLPCC-700	1028.7	0.75	0.35	0.32	46.7	42.7	2.58
PLPCC-800	1175.6	0.87	0.41	0.36	47.1	41.4	2.57

S_{BET}: Specific surface area was determined using the Brunauer-Emmett-Teller (BET) equation.
V_{total}: Total pore volume was determined by NLDFT model.
V_{mic}: Micropore volume was determined by NLDFT model.
V_{meso}: Mesopore volume was determined by NLDFT model.

Table S3 Specific capacities of PLPCCs tested under the current density of 0.2 and 1 $A·g^{-1}$.

Electrodes	Specific capacity ($mAh·g^{-1}$)			
	0.2 $A·g^{-1}$		1 $A·g^{-1}$	
	25th	200th	100th	600th
SLCM	235.1	256.1	165.0	209.7
PLPCC-600	455.5	543.2	322.9	386.5
PLPCC-700	642.5	706.3	436.9	530.4
PLPCC-800	445.8	618.5	289.3	448.7

Table S4 Comparison of lithium storage performance of PLPCC-700 with different carbonaceous materials in the reported literatures.

Materials	Specific surface area ($m^2·g^{-1}$)	ICE[a] (%)	Cycling data[b]	Rate capacity[c]	Ref.
PLPCC-700	1029	49.2	706/200/200	530/1000	This work
Hierarchical porous carbon (HPC)	420	40.4	390/50/37	266/1860	[1]
Hierarchical porous carbon (LHPC)	907	41.6	470/275/200	268/1000	[2]

Hierarchical porous carbon ($HLPC-ZnCO_3-600$)	531	54.9	550/200/200	315/1000	[3]
Hierarchical porous carbon (KHPC-600)	735	47.3	650/60/100	346/5000	[4]
Macroporous carbon (MPC-3)	631	54.3	501/120/200	306/1000	[5]
Nanoporous hard carbon microspheres (NHCS-6)	753	45.0	230/30/100	157/1490	[6]
Carbon nanofibers/nanosheets hybrid (CNFS)	847	-	592/200/100	508/1000	[7]
Graphene aerogels (GA)	530	-	439/30/100	250/1000	[8]
N-doped carbon nitride (CNNC)	-	-	430/60/50	323/2500	[9]

[a] Initial coulombic efficiency

[b] Capacity ($mAh\cdot g^{-1}$)/cycle numbers/current density ($mA\cdot g^{-1}$)

[c] Capacity ($mAh\cdot g^{-1}$)/current density ($mA\cdot g^{-1}$).

References

[1] J. Yang, X. Y. Zhou, Y. L. Zou and J. J. Tang, *Electrochim Acta*, 2011, **56**, 8576-8581.
[2] W. L. Zhang, J. Yin, Z. Q. Lin, H. B. Lin, H. Y. Lu, Y. Wang and W. M. Huang, *Electrochim Acta*, 2015, **176**, 1136-1142.
[3] Y. B. Xi, S. Huang, D. J. Yang, X. Q. Qiu, H. J. Su, C. H. Yi and Q. Li, *Green Chem*, 2020, **22**, 4321-4330.
[4] D. P. Qiu, C. H. Kang, M. Li, J. Y. Wei, Z. W. Hou, F. Wang and R. Yang, *Carbon*, 2020, **162**, 595-603.
[5] Y. X. Fu, X. Y. Pei, D. C. Mo and S. S. Lyu, *J Mater Sci-Mater El*, 2019, **30**, 5092-5097.
[6] S. M. Jafari, M. Khosravi and M. Mollazadeh, *Electrochim Acta*, 2016, **203**, 9-20.
[7] S. B. Wang, C. L. Xiao, Y. L. Xing, H. Z. Xu and S. C. Zhang, *J Mater Chem A*, 2015, **3**, 6742-6746.
[8] Y. X. Xu, Z. Y. Lin, X. Zhong, B. Papandrea, Y. Huang and X. F. Duan, *Angew Chem Int Edit*, 2015, **54**, 5345-5350.
[9] W. L. Zhang, J. Yin, C. L. Chen and X. Q. Qiu, *Chem Eng Sci*, 2021, **241**, 116709.