physchem

Supporting Information

Effect of Silicon Crystal Size on Electrochemical Properties of Magnesium-Doped SiOx Anode Materials for Lithium-Ion Batteries

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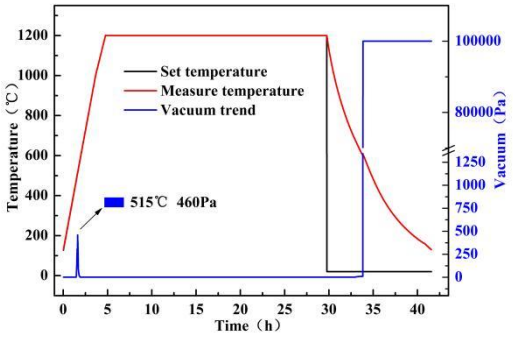

Figure S1. Temperature Profile of the Preparation Process (Example of 1200 °C Constant Temperature, with Pressure Curve).

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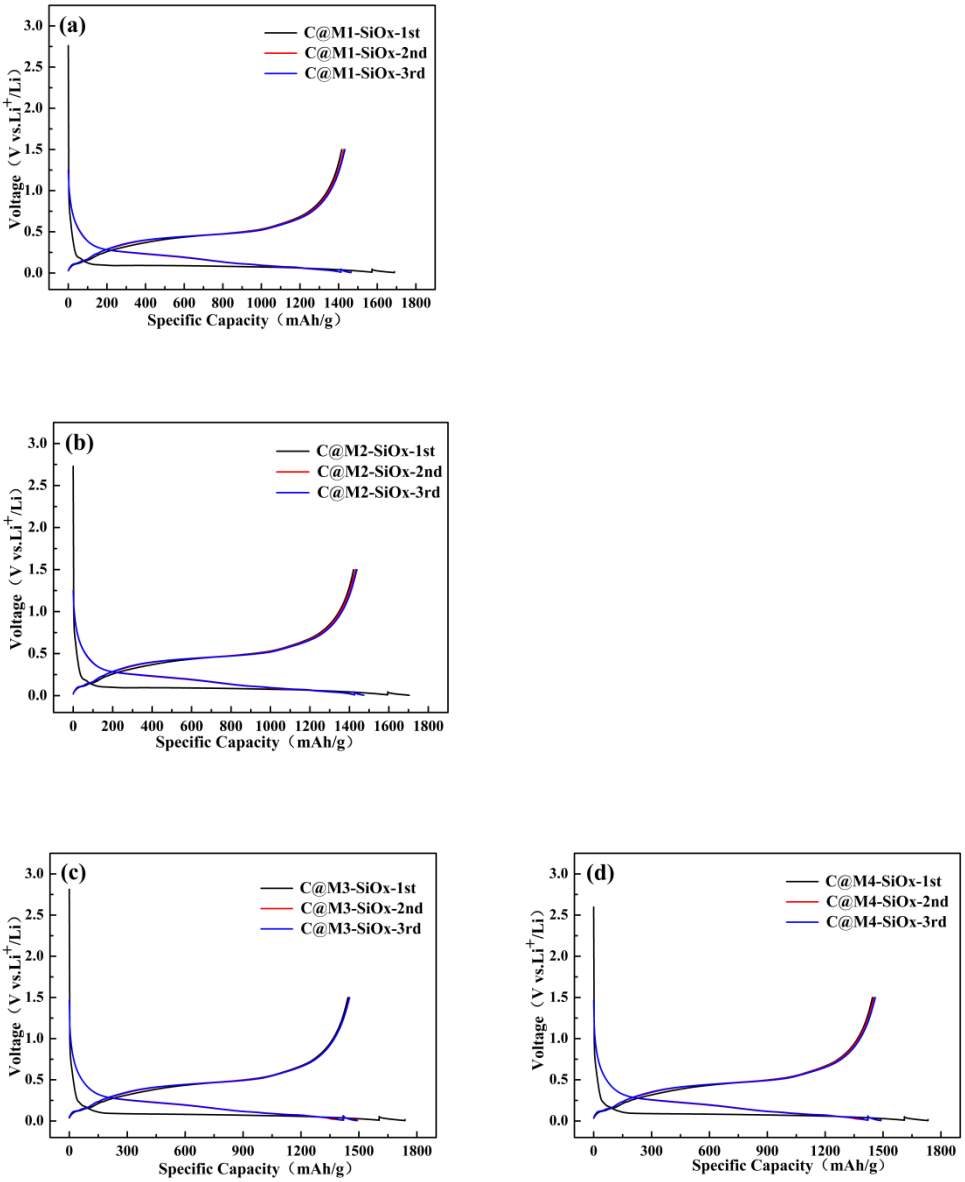

Figure S2. Voltage-Capacity Profiles of C@M-SiOx: (a) C@M1-SiOx,(b) C@M2-SiOx,(c) C@M3-SiOx,(d) C@M4-SiOx.

Table S1. The de-lithiation specific capacity, lithiation specific capacity and Coulombic efficiency of the C@M-SiOx sample during the first three cycles.

Electrodes	Lithiation Specific Capacity（mAh/g）			Delithiation Specific Capacity（mAh/g）			Coulombic Efficiency（%）		
	1st	2nd	3rd	1st	2nd	3rd	1st	2nd	3rd
C@M1-SiOx	1729.1	1464.2	1463.8	1418	1426.1	1433.1	82.01	97.4	97.9
C@M2-SiOx	1722.9	1472.4	1472.8	1429	1431.2	1437.4	82.94	97.2	97.6
C@M3-SiOx	1730.5	1489.1	1486.7	1442	1453.4	1459.9	83.33	97.6	98.2
C@M4-SiOx	1713.8	1460	1459.6	1431	1422	1430.4	83.5	97.4	98.0

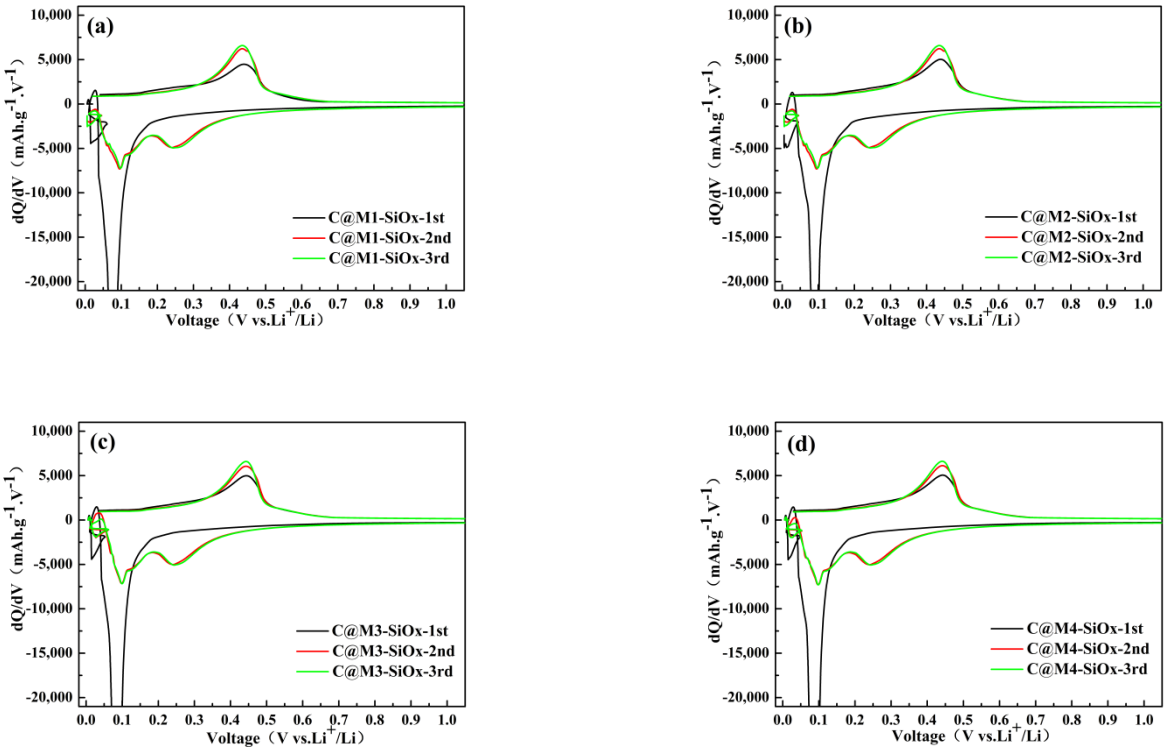

Figure S3. dQ/dV Curves of C@M-SiOx:(a) C@M1-SiOx,(b) C@M2-SiOx,(c) C@M3-SiOx,(d) C@M4-SiOx.

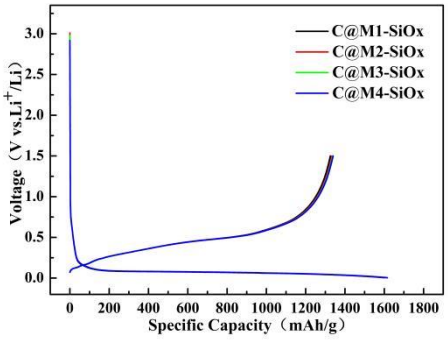

Figure S4. Voltage-Capacity Profiles of C@M-SiOx: (a) C@M1-SiOx,(b) C@M2-SiOx,(c) C@M3-SiOx,(d) C@M4-SiOx.

Table S2. Comparison of initial capacity and efficiency under the conventional charge-discharge mechanism (0.1C).

Electrodes	Lithiation Specific Capacity（mAh/g）	Delithiation Specific Capacity（mAh/g）	Initial Coulombic Efficiency（%）
C@M1-SiOx	1325.5	1599.2	82.89
C@M2-SiOx	1333.1	1607.7	82.92
C@M3-SiOx	1347.4	1621.1	83.12
C@M4-SiOx	1349.5	1623.1	83.14

Table S3. Performance comparison of SiOx-based materials obtained via different preparation methods and modification techniques.

Materials	Method/ structure	Current Density /Capacity(mAh g^{-1}) /Cycle Number (n) /capacity retention(%)	Initialcapacity ($mAhg^{-1}$) /ICE(%)	Maximum rate /Capacity($mAhg^{-1}$) /Cycle Number (n)	Ref.
D-SiO@G	Solution-ball milling-heat treatment	2A g^{-1}/1097/500/72.4	1515.2/78.20	5A g^{-1}/774/10	[20]
SiOx/C	Template-free aldimine condensation	0.1A g^{-1}/650/100/60.29	1078/65.3	1A g^{-1}/469/1000	[21]
m-SiOx@C/MXene	situ carbon coating and electrostatic self-assembly	0.2A g^{-1}/1150/100/62.46	1423.1/77.3	2A g^{-1}/628/8	[22]
SiOx/C	magesiothermic reaction , hot-water treatment	0.8A g^{-1}/550/200/78.81	620/87.49	3A g^{-1}/380/10	[23]
SiO/TiO_2–x	chemical etching, hydroly-sis	1 A g^{-1}/501.2/300/52.41	1098.7/65	2A g^{-1}/345.9/10	[24]
$SiO_{0.4}$/CNTs@C	thermal plasma	0.2 A g^{-1}/1993/300/96.84	2058/81.9	3A g^{-1}/1440/2000	[25]
SiOx@$Li_{0.75}$PAA	engineering prelithiation binder	0.2 A g^{-1}/871/170/58.7	1485/67.5	4C/221/10	[26]
SiOx/C@CNTs	the sol–gel method, poly-mer coating	0.1 A g^{-1}/702/200/76.22	921/64.6	0.5 A g^{-1}/511/450	[27]
Fe–SiOx@C	Fe^{2+} modification, carbon coating	0.5A g^{-1}/552.4/500/64.91	851/57.8	2 A g^{-1}/354/-	[28]
SiOx@TiON-C	solvothermal and thermal reduction	0.5 A g^{-1}/750/500/50	1000/75.1	3C/455/10	[29]
V–SiOx@AP@C	vacuum thermal re-duced，double-coating layers	1 A g^{-1}/761.5/200/42.8	1775.8/87.6	2 A g^{-1}/820/10	[30]
SiOx/vG-F	surface fluorination，ver-tical graphene carbon shells	0.5C/1548.6/150/87.6	1593.1/75.3	5C/1471.8/5	[31]
SiO–SiO_2@C	liquid-phase method	0.2 A g^{-1}/1061/100/97	1566.6/75.73	3 A g^{-1}/703/10	[32]
PBC-x(Li$_x$SiO_y Matrix)	disproportionation reac-tion,chemical vapor depo-sition	0.4 A g^{-1}/668/100/67.2	994.6/82.6	-	[33]