Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

A three layer design with mesoporous silica encapsulated by carbon core and shell for high energy Lithium ion battery anode

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Supporting Information

1. Theoretical capacity of SiO_2

According to previous study, it can be summed that three types of reaction exist between silica and Li ions. According to these reaction equations, the theoretical capacity of SiO_2 can be calculated based on the number of transfer electrons and shown in Table. S1[1,2]. The theoretical capacity of SiO_2 increases with the reduction of the amount of silica. Namely, the reaction generated Li_2O and Si shows the largest reversible capacity of 1961 $mAhg^{-1}$.

The calculation should be:

Weight of 1 Mole of SiO_2: 60g

Coulombs in 1 Mole (one charge per Li): 96 485*4 .4

Coulombs in 1 mAh: 3.6

mAh per mole of charge: 96 485*4.4 /3.6= 117925

mAh per gram of SiO_2: 117925/60.08 = 1961 $mAhg^{-1}$

Table. S1: The theoretical capacities and the molar ratios of SiO_2 and Li ions in different mechanisms[3]

Mechanism	Reaction equations	The molar ratio of SiO_2 and Li ions	Theoretical initial capacity of SiO_2	Theoretical reversible capacity of SiO_2
1	$5SiO_2+4Li^++4e\leftrightarrow 2Li_2Si_2O_5 + Si$ $Si + 22Li^+ + 22e \leftrightarrow Li_{22}Si_5$	5:4	749 $mAhg^{-1}$	749 $mAhg^{-1}$
2	$2SiO_2+4Li^++4e\rightarrow Li_4SiO_4+ Si$ $5Si+22Li^++ 22e \leftrightarrow Li_{22}Si_5$	1:2	1872 $mAhg^{-1}$	980 $mAhg^{-1}$
3	$SiO_2+4Li^++4e\rightarrow 2Li_2O + Si$ $5Si+22Li^++22e \leftrightarrow Li_{22}Si_5$	1:4	3744 $mAhg^{-1}$	1961 $mAhg^{-1}$

However, it is reported that the reversible reaction of $Li_2Si_2O_5$ (Mechanism 1) and the irreversible reaction of both Li_2O (Mechanism 3) and Li_4SiO_4 (Mechanism 2) are coexistence in the electrochemical reaction between silica and Li ions[3,4].

1. Q. Sun, B. Zhang and Z. W. Fu, *Appl. Surf. Sci.*, 2008, **254**, 3774-3779.
2. B. K. Guo, J. Shu, Z. X. Wang, H. Yang, L. H. Shi, Y. N. Liu and L. Q. Chen, *Electrochem Commun*, 2008, **10**, 1876-1878.
3. N. Yan, F. Wang, H. Zhong, Y. Li, Y. Wang, L. Hu and Q. W. Chen, *Scientific Reports*, 2013, **3**, 6.
4. W. S. Chang, C. M. Park, J. H. Kim, Y. U. Kim, G. Jeong and H. J. Sohn, *Energy & Environmental Science*, 2012, **5**, 6895-6899.

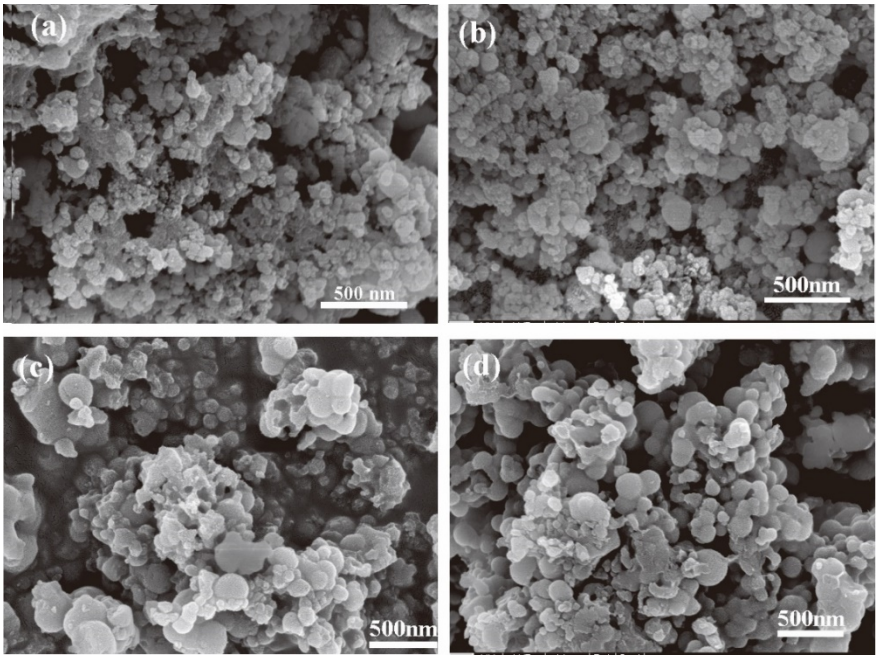

Fig. S1 The general view of mcms (a), C-mcms (b), ms(c), and C-ms (d)

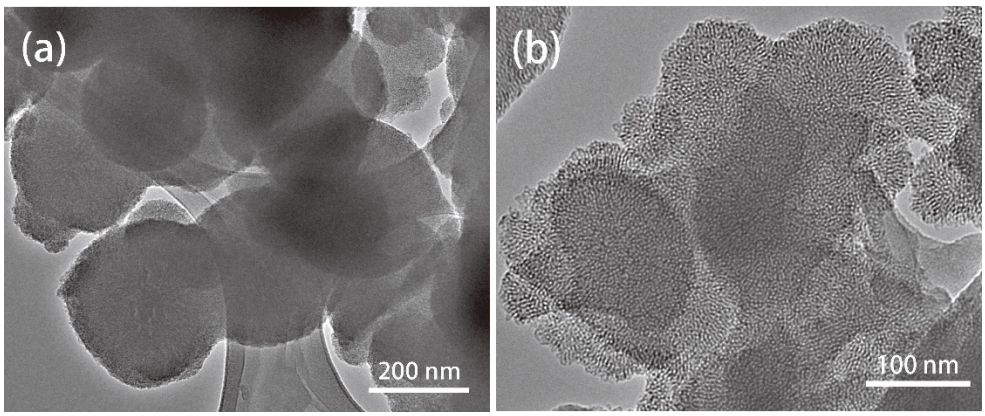

Fig. S2 TEM images of the mcms (a) and C-ms (b)

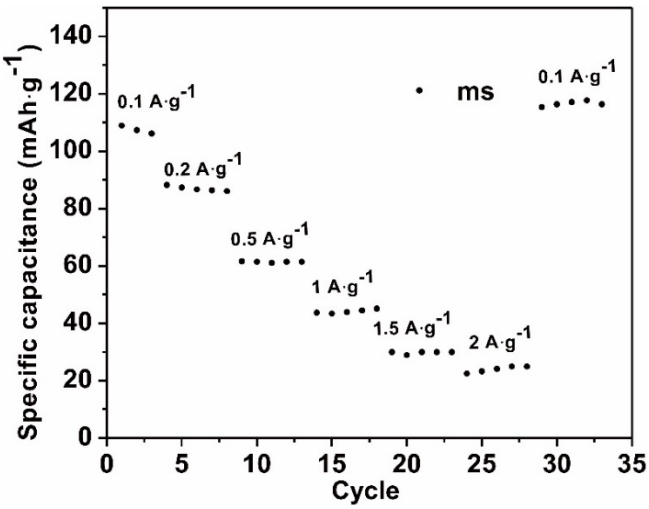

Fig. S3 Rate performance of mesoporous silica.