Rigid TiO$_{2-x}$ Coating on Mesoporous Hollow Si Spheres with High Structure Stability for High Performance Lithium-Ion Battery

Yongli Yu$^a$, Xu Chen$^a$, Wensheng Yang$^a$, Junfeng Rong$^b$

$^a$State Key Laboratory of Chemical Resorcr Engineering, Beijing University of Chemical Technology, Beijing, 100029, China

$^b$The State Key Laboratory of Catalytic Material and Reaction Engineering, Sinopec Research Institute of Petroleum Processing, Beijing, 100029, China

E-mail: rongjf.ripp@sinopec.com

High–energy–density Li–ion batteries with long–cycle and high–rate performances are in great demand for the development of electric vehicles [1, 2]. Silicon is regarded as a potential alternative to commercially used graphite due to its high theoretical capacity (4200 mAh·g$^{-1}$). Unfortunately, particle pulverization resulting from the tremendous volume change during operation and inherently low electrical conductivity seriously limit its electrochemical performance and large-scale application.

In this work, we developed a facile approach for the fabrication of mesoporous hollow silicon spheres@TiO$_{2-x}$ (MHSi@TiO$_{2-x}$) nanocomposite through the magnesiothermic reduction of hollow silica nanospheres, in situ tetrabutyltitanate hydrolysis on the MHSi surface, and sequent calcination in inert atmosphere.

**Results and Discussion**

As shown in Figure 1, the mesoporous hollow structure can be clearly observed, and the mesoporous Si is surrounded by a uniform TiO$_{2-x}$ coating layer. At a current density of 2 A·g$^{-1}$, MHSi@TiO$_{2-x}$ delivers a high reversible specific capacity of 1303.1 mAh·g$^{-1}$, and 84.5% capacity retention after 500 cycles.

![Figure 1. (a,b) HRTEM images of the MHSi@TiO$_{2-x}$ composite, (c) Cyclic performance of MHSi and MHSi@TiO$_{2-x}$ at 2 A·g$^{-1}$.](image)

**Conclusion**

In summary, an interface-engineered Si-based anode with a mechanically and electrically robust structure has been synthesized via a facile method. The conductive TiO$_{2-x}$ shell not only enhances the transport kinetics of electron and Li$^+$, but also provides a rigid structure with high mechanical stability to confine the outward expansion of Si, maintaining the structural integrity and a stable SEI. The mesoporous hollow structure provides enough void space for expansion of Si, effectively buffering large volume change. As a result, MHSi@TiO$_{2-x}$ anode yields excellent cycling stability and superior rate capability.

**References:**
