Dual-functionalized double carbon shells coated silicon nanoparticles for high performance lithium ion batteries

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Abstract  
To address the challenge of huge volume change and unstable solid electrolyte interface (SEI) of silicon in cycles,\textsuperscript{1-4} causing severe pulverization, we propose a “double-shell” concept. This concept is designed to perform dual functions on encapsulating volume change of silicon and stabilizing SEI layer in cycles using double carbon shells. Double carbon shells coated Si nanoparticles (DCS-Si) are prepared. Inner carbon shell provides finite inner voids to allow large volume changes of Si nanoparticles inside of inner carbon shell, while static outer shell facilitates the formation of stable SEI. Most importantly, inter-shell spaces are preserved to buffer volume changes and alleviate mechanical stress from inner carbon shell. DCS-Si electrodes display a high rechargeable specific capacity of 1802 mAh g\textsuperscript{−1} at a current rate of 0.2 C, superior rate capability and good cycling performance up to 1000 cycles. A full cell of DCS-Si/LiNi_{0.45}Co_{0.1}Mn_{1.45}O_4 exhibits an average discharge voltage of 4.2 V, a high energy density of 473.6 Wh kg\textsuperscript{−1}, and good cycling performance. Such double-shell concept can be applied to synthesize other electrode materials with large volume changes in cycles by simultaneously enhancing electronic conductivity and controlling SEI growth.

Double carbon shell-encapsulated Si nanoparticles (DCS-Si) perform dual functions, which deliver a high reversible capacity of 1802 mAh g\textsuperscript{−1} at 0.2 C, superior rate capability, and cyclability (1000 cycles). Full cell of DCS-Si/LiNi_{0.45}Co_{0.1}Mn_{1.45}O_4 exhibits high energy density of 473.6 Wh kg\textsuperscript{−1}, and good cyclability with a capacity retention of 93.8%.

References:  