2nd World Congress and Expo on
Nanotechnology and Material Science
April 04-06, 2016 at Dubai, UAE

Interfacial Lithium Storage in Graphene/Metal Oxide and Sulphide

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Graphene/metal oxide and sulphide nanocomposites have been widely studied as anode materials for lithium ion batteries and exhibit excellent electrochemical properties, due to the synergistic effect between graphene and metal oxide and sulfide. Based on the first-principles total energy calculations, it is revealed that interfacial oxygen atoms play an important role on the interfacial lithium storage of G/TiO_2. Surface and interfacial lithium storage via an electrostatic capacitive mechanism contributes significantly to the electrode capacity. In graphene/metal sulphide nanocomposites, Li adsorption energies at interfaces are larger than that on the corresponding metal sulphide surfaces with almost no enhancement of the energy barriers for Li atom diffusion. The enhanced Li adsorption capability at Li_2S/G interface contributes to the extra storage capacity of graphene/metal sulphide composites. Thereby, a smart composite consisting of sandwich-like nanosheets with uniform MoS_2@ carbon-coated ultrathin TiO_2 nanosheets has been constructed through facile hydrothermal method to enhance the cycling and rate performances of MoS_2. In this uniform sandwich-like structure, carbon-coated ultrathin TiO_2 is conformably embedded by MoS_2 shells *via* intimate interfacial contacts, while the carbon coats TiO_2 *via* Ti-O-C bonds. Due to the abundant interfaces in the composites, as well as the high structure stability of TiO_2 during charge and discharge cycles, high-performance of the lithium-ion battery anode material is obtained.

Biography:

Enzuo Liu is an associate professor at school of materials science and technology of Tianjin University (China). Prior to joining TJU in 2009, he completed his Ph.D. in physics at Tsinghua University (China), in 2007, and worked in Prof. Jianzhong Jiang's group at Zhejiang University (China) as postdoc. His research aims at improving the nanocomposites properties through interface engineering.