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Surface chemistry and electrode design for high performance Li-S batteryWen Liu¹, Cejun Hu¹, Jijin Yang¹, Qian Wang², Kai Wu² and Xiaoming Sun¹¹Beijing University of Chemical Technology, China²Peking University, China

Based on the reaction of $16\text{Li} + \text{S}_8 \leftrightarrow 8\text{Li}_2\text{S}$, Li-S battery reaches a high theoretical energy density of 2600 Wh/kg, which is several times higher than that of traditional lithium ion batteries (LIBs). The low cost, high capacity as well as environment-benignity makes Li-S battery as a strong candidate for next generation energy storage. However, the development of Li-S battery is severely hindered by several problems, including the low conductivity of sulfur cathode, volume variation during charge/discharge and dissolution of lithium polysulfide (LiPS). These drawbacks cause low utilization of sulfur and poor cycling performance of batteries. To overcome these obstacles, researchers pay attention to regulating the construction of sulfur cathode, using mesoporous materials, core-shell types carbon and graphene oxide etc. The carbon based materials have significant benefit on the conductivity of the electrode and suppress the polysulfide dissolution to some extent. But the nonpolar carbon intrinsically has poor interaction with LiPS and lithium sulfide. Moreover, the lithium dendrite growth and electrode pulverization during cycling gives rise to lower columbic efficiency and safety risks. Hence, the polysulfide trapping chemistry, sulfur electrode design and Li metal electrode protection are the key factors contributing to the cycling performance and stability of Li-S battery. Herein, we propose polar materials including inorganic metal oxides, metal phosphides and organic functional groups, which further hybrid with nano carbons to construct bifunctional host for sulfur electrode. On one hand, the polar sites can strongly absorb LiPS, so that the dissolution of LiPS and shuttling effect can be reduced. On the other hand, polysulfide after absorption can quickly reacted with electrons and Li-ions, therefore improving the reaction kinetics and eliminating the bulky dead sulfur formation. Consequently, the Li-S batteries with the high performance sulfur electrodes can stably run for over 1000 cycles. The mechanism of sulfur trapping chemistry was also revealed by x-ray photoelectron spectroscopy (XPS) characterization and theoretical calculation. In terms of Li metal anode, the huge volume variation during cycling cause electrode pulverization, which is especially serious when paired with high mass loading sulfur cathode. We demonstrate that nanostructuring is one of the key points to realize stable lithium metal anode. Different kinds of scaffold have been constructed with Li metal to reduce the volume variation and suppress dendrite growth. The lithiophilic treatment of scaffold leads to lithium uniformly deposit and nucleate on electrode surface. The dendrite-free lithium deposition also achieved through manipulation of Li-ions transport number by modifying a separator with metal-organic framework materials (MOFs).

Recent Publications

1. C Milroy and A Manthiram (2016) *Adv. Mater.*, 28.
2. Y Y Mi, W Liu, K R Yang, J Jiang, Q Fan, Z Weng, Y R Zhong, Z S Wu, G W Brudvig, V S Batista, H H Zhou and H L Wang (2016) *Angew. Chem. Int. Ed.*, 55:14818-14822.
3. W Liu, J Jiang, Y Y Mi, K Yang, Z Weng, Q Fan, V S Batista, G Brudvig and H L Wang (2017), DOI: 10.1073/pnas.1620809114.
4. Y Zhong, K R Yang, W Liu, P He, V S Batista and H L Wang (2017) *J. Phys. Chem. C*, 121:14222-14227.
5. W Liu, Z Weng, Y Y Mi and H L Wang (2017) *Chem. Sci.* 8:4285-4291.

Biography

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