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Metal-organic Framework Glass Anodes for Li-ion Batteries

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Abstract: Metal-organic frameworks (MOFs) hold great promise as high-energy anode materials for advanced lithium-ion batteries (LIBs) owing to their great porosity, abundant reaction sites, tunable structures [1]. However, the pore structure of crystalline MOFs tends to collapse during the charge-discharge cycling, significantly degradating their electrochemical performances. In contrast, the recently discovered zeolitic imidazolate framework (ZIF) glasses exhibit different structural features, e.g., high degree of short-range disorder [2], with retained porosity. As a critical breakthrough, we prepared the first MOF (Cobalt-ZIF-62) glass anode by melt-quenching for LIBs, which exhibits high specific capacity (306 mAh g^{-1} after 1000 cycles at 2 A g^{-1}), outstanding cycling stability, and superior rate performance compared with the crystalline Cobalt-ZIF-62 and the amorphous one prepared by high-energy ball-milling [3]. To further improve the electrochemical performances of Cobalt-ZIF-62 glass anode, we present a strategy to in situ grow it on the surface of Si nano particles, and then to transform the thus-derived material into Si@ZIF-glass composite (SiZGC) through melt-quenching. The electrochemical characterizations of SiZGC show that proper tuning the Si loading in cobalt-ZIF-62 can lead to a considerable enhancement in discharge capacity up to ~650 mA h g^{-1}, which is about three times that of ptistine ZIF glass at 1 A g^{-1} after 500 cycles [4]. More impressively, the capacities of both the pristine ZIF glass and the SiZGC anodes continuously rise with charge-discharge cycling and even tripled after 1000 cycles. Through both the structural characterizations and density functional theory calculations, we revealed that their cycling-induced enhancement of the performances originate from the increased distortion and local breakage of the Co-N coordination bonds, making the Li-ion intercalation sites more accessible.

Additionally, the ZIF glass phase in SiZGC can not only contribute to lithium storage, but also buffer the volume changes and prevent the aggregation of Si nano particles during lithiation/delithiation processes.

Key words: Metal-organic framework glass; Anode; Silicon; Lithium-ion batteries

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