Accepted Manuscript

Systematic post-synthetic modification of metal-organic framework (ZIF-67) with superior cyclability for lithium-ion batteries

Weiyang Li, Fan Yang, Xujun Fang, Yichuan Rui, Bohejin Tang

PII: S0013-4686(18)31354-9

DOI: 10.1016/j.electacta.2018.06.066

Reference: EA 32059

To appear in: *Electrochimica Acta*

Received Date: 23 April 2018

Revised Date: 8 June 2018

Accepted Date: 9 June 2018

Please cite this article as: W. Li, F. Yang, X. Fang, Y. Rui, B. Tang, Systematic post-synthetic modification of metal-organic framework (ZIF-67) with superior cyclability for lithium-ion batteries, *Electrochimica Acta* (2018), doi: 10.1016/j.electacta.2018.06.066.

Systematic Post-synthetic Modification of Metal-Organic Framework (ZIF-67) with Superior Cyclability for Lithium-ion Batteries

Weiyang Li, Fan Yang, Xujun Fang, Yichuan Rui and Bohejin Tang*

College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China

* Corresponding author: tangbohejin@sues.edu.cn

Abstract

In this work, carboxyl groups were introduced on the organic ligands of ZIF-67 through post-synthetic modification (-CH_3→-CH_2Br→-CHO→-COOH). A thin layer of Ag nanoparticles (3 nm in diameter) coating was deposited on external surface of ZIF-67 crystals through the reaction between the aldehyde groups in the ligands and silver ammonia solution. The carboxyl groups can participate in the lithium storage while the Ag nanoparticles coating help in increasing the conductivity. Electrochemical properties of the modified ZIF-67 electrodes are examined by cyclic voltammetry and galvanostatic charge/discharge tests. Benefiting from the outstanding conductivity of Ag nanoparticles and the synergistic effect between Ag nanoparticles and the modified ZIF-67, the composite exhibits enhanced electrochemical performance compared to its ZIF-67 counterpart. Nearly an invariable capacity of 800 mA h g^{-1} is maintained up to 100 cycles at 0.28 C (1C=137 mA g^{-1}) with a Coulombic efficiency of 99%. Furthermore, the ex situ X-ray diffraction and X-ray photoelectron spectroscopy studies on the electrode material under different