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Synthesis, crystal structure of a lithium - zinc bimetal coordination polymer and its graphene composite as anode materials for lithium ion battery

Jipeng Tan, ¹ Fa-Nian Shi, * ¹ Fang Hu, ² Gui-Mei Shi, ¹ Bo Tian * ¹ and Hongpeng You ³

¹School of Science, Shenyang University of Technology, Shenyang 110870, P.R. China.

²School of Materials Science and Engineering, Shenyang University of Technology.

³State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P.R. China.

*E-mail: shifn@sut.edu.cn; tian-harry@foxmail.com

Abstract: A new bimetal coordination polymer composed of Li⁺, Zn²⁺ and 4,5-imidazole dicarboxylic acid (idca) with a molecular formula of Li₅Zn₆C₂₅H₁₁N₁₀O₂₄ (LiZn1) was prepared via a simple hydrothermal method. The single crystal structure shows that LiZn1 has a 3-D framework consisting of three independent four coordinated Li⁺ and three independent five coordinated Zn²⁺ cations, respectively. Topological study indicates the network of LiZn1 is 9-nodal, 3,3,3,3,3,4,5,5,6-connected net, with a point symbol of $\{4.6.7\}_2\{4.6^2\}_4\{4^2.6^2.7^2.9^3.11\}\{4^2.6\}_2\{4^3.6^3.7^2.8^5.9^2\}_2\{4^3.6^3\}_2\{6^2.8\}\{6^5.7^2.8.9^2\}_2$.

The graphene composite (LiZn1/gr) was prepared via a sonication treatment of the mixture of LiZn1 and graphene. LiZn1 was employed as the anode of a lithium ion battery, the initial discharge capacity was obtained for 558 mAh/g, after 100 cycles the discharge capacity was decreased to around 75 mAh/g. However, the graphene composite (LiZn1/gr) has improved very much the performance with the initial discharge capacity of 1090 mAh/g and after 100 cycles the discharge capacity could remain about 133 mAh/g.

Keywords: Lithium; Zinc; Coordination polymer; Lithium ion battery; Capacity; Anode material

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