Enhanced Electrochemical Performance Ru³⁺ Doped Li₂FeP₂O₇ as Cathode for Lithium Ion Batteries

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Li₂Fe_{1-x}Ru_xP₂O₇ (x = 0, 0.005, 0.01, 0.02, 0.03, and 0.04) were prepared by a simple sol-gel synthesis method. Detailed lattice information, including the observation of a monoclinic P2₁/c (14) space group and crystal structure, was determined using XRD with rietveld refinement. To further confirm the oxidation and chemical states of elements within the samples, XPS measurements of each element are used. The electrochemical measurements were conducted using EIS, CV, and galvanostatic charge-discharge testing. Li₂Fe_{0.99}Ru_{0.01}P₂O₇ exhibited an increased specific discharge capacity of 100.22mAh/g at 0.05C and decreased polarization during charge and discharge. Li₂Fe_{0.99}Ru_{0.01}P₂O₇ exhibited the best rate-capabilities at various current densities, as well as the best cycle abilities in the voltage range of 2.0-4.5V. Fe K-edge and Ru K-edge in-situ XAS were carried out for samples of Li₂FeP₂O₇ and Li₂Fe_{0.99}Ru_{0.01}P₂O₇ in order to observe changes in the structures of the materials during electrochemical reaction. The results indicate that the structural rearrangement of Li₂Fe_{0.99}Ru_{0.01}P₂O₇ might be reduced by the slight shrinkage of the lattice due to the “pillar effects” of Ru³⁺. Also, Li₂Fe_{0.99}Ru_{0.01}P₂O₇ demonstrated higher electronic conductivity and ionic diffusion coefficient than Li₂FeP₂O₇. Therefore, the higher electrochemical performance of Li₂Fe_{0.99}Ru_{0.01}P₂O₇ was related with structure stability, electronic conductivity, and ionic diffusion coefficient.

Keywords: Lithium ion batteries, Cathode, Lithium iron pyrophosphate, Ru-doping, pillar effect

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