Int. J. Electrochem. Sci., 16 **(2021)** Article Number: 211226, doi: 10.20964/2021.12.11

International Journal of
ELECTROCHEMICAL
SCIENCE
www.electrochemsci.org

Mini Review

Recent Advances in $LiFePO_4$ Cathode Materials for Lithium-Ion Batteries. First-Principles Research

Qun-fang Zhao[1,2,3,&], *Shu-qiong Zhang*[1,2,3,&], *Min-yi Hu*[1,2,3], *Chang Wang*[1,2,3], *Guang-hui Jiang*[1,2,3,*]

[1] Advanced Batteries and Materials Engineering Research Center, Guizhou Light Industry Technical College, Guiyang 550025, China;
[2] Graphene Materials Engineering Research Center of Guizhou Colleges and Universities, Guiyang 550025, China;
[3] Provincial Collaborative Innovation Center of Used Power Batteries Recycling, Guiyang 550025, China;
& These authors contributed equally to this work and should be considered co-first authors
[*]E-mail: jianggh88@foxmail.com

Received: 2 September 2021 / *Accepted:* 30 September 2021 / *Published:* 10 November 2021

Lithium-ion batteries (LIBs) are the dominant battery technologies from portable electronics to electronic vehicles due to their high energy density and excellent cycling performance. The discovered $LiFePO_4$ cathode with good cycling stability, low price and excellent safety is one of the most attractive cathode materials for LIBs. However, several crucial challenges including poor ionic and electronic conductivity and low Li^+ diffusion impede its high-rate application. To improve these troublesome issues, many investigations have been performed, and the electrochemical performance of $LiFePO_4$ has been enhanced. However, the modified origins of the electronic structure and ionic dynamic properties of $LiFePO_4$ cathodes are still being explored. Computational research provides a better understanding of the above improvements to a significant extent. In this review, recent achievements in first-principles studies of $LiFePO_4$ cathode materials are discussed, including structure, electronic properties, Li-ion transport characteristics, mechanical stability and thermodynamic properties.

Keywords: Lithium-ion batteries; $LiFePO_4$; First-principles; Advances

FULL TEXT