ABSTRACT

Report: 29 pages, 7 figures, 1 table, 30 references.

Purpose: Simulation $LiFePO_4$ structures, valuation, based on the calculations, the possibility of their further use in lithium power sources.

The object of study: System $LiFePO_4$.

Methods: Studies were carried out using quantum-chemical modeling software package licensed in Virtual NanoLab within density functional method (DFT).

Practical value: The model can be used to develop new cathode materials for lithium batteries.

The results and their novelty: Our studies indicate that the accumulation of lithium on the surface is the cause of its slow diffusion, namely limiting stage of transition from surface to subsurface layers. The results determine the direction of future research in this area.

$LiFePO_4$, DESIGN, VIRTUAL NANOLAB, DENSITY FUNCTIONAL THEORY, METHOD OF ELASTIC TAPES, DIFFUSION