ABSTRACT

Diploma work: 75 pages, 12 figures, 10 table, 49 references.

The aim of the study: modeling structure to hold $LiFePO_4$ based on the first principle; calculate the diffusion coefficient and diffusion activation energy lithium atom in the bulk and on the surface.

The methods of the study: draft functional theory (DFT), nudged elastic band (NEB), generalized gradient approximation (GGA).

The object of study: system $LiFePO_4$.

Scientific novelty: studies suggest that the reasons for the slow diffusion of lithium in the structure of $LiFePO_4$ are a number of factors that related to its structure. The results determine the direction of future research in this area.

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

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