

## ABSTRACT

Report: p. 29, fig. 5 table 2, sources 37.

Research object – single-component thin-film  $\text{Me}_1$  and  $\text{Me}_2$ , multi-component  $\text{Me}_1\text{-Me}_2$  and  $\text{Me}_2\text{-Me}_1$ .

Purpose is to determine the thermodynamic and diffusion characteristics of the systems based on density functional theory.

Research methods – computer simulation, based on density functional theory implemented via VASP software.

The novelty of the work lies in the implementing of the first-principle methods with quasiharmonic approximations to study the diffusion barriers of the front contacts of silicon solar cells.

Results of this work can be used in the field of energetic, in the process of manufacture of solar cells.

**KEYWORDS: SOLAR CELL FRONT CONTACT, DIFFUSION BARRIER, SELF-DIFFUSION, HETERODIFFUSION, FIRST-PRINCIPLE SIMULATION**