ABSTRACT

Attestation bachelor work: 71 pages, 42 figures, 8 tables, 38 literature sources

Purpose of the study: featuring the first principle approach to simulate the crystal structure of topological insulator for example Bi_2Se_3 and analyze the band structure of the material for the zones that do not overlap in scope and areas that overlap on the surface.

Object of the study: topological insulator for example Bi_2Se_3.

Methods: Ab–initio calculations and density functional theory with the software package Virtual NanoLab.

Scientific innovation: confirmed that the structure is Bi_2Se_3 topological insulator, which in bulk is an insulator and conductor on the surface, due to tight correlation between the electron and its spin direction of the electrons are not scattered on surface inhomogeneities obtained data do not differ from experimental.

Practical application: the results have practical made in the topological insulator and further, and the given approach can be used to search for new materials that would have the properties of topological insulators.

TOPOLOGICAL INSULATOR; VIRTUAL NANOLAB; FUNCTIONAL THEORY DENSITY; MODELING; BI2SE3; APPROACH KOHN-SHAM; FIRST PRINCIPLE CALCULATIONS