

ABSTRACT

Diploma work: 69 pages, 25 figures, 5 tables, 10 sources of information.

GRAPHEN, MODELING NANOSISTEM, SOFTWARE.

Object of research – graphene planes.

The purpose of the work is to model the graphene nanostructure and calculate it using a software application such as Virtual Nanolab.

The basis of the computational experiment is the research of computer models at different values of the input parameters, the theoretical basis of the models used in this paper – physical material science, applied mathematics and mathematical modeling, and technical – powerful electronic computers and specialized software.

The use of a computational experiment as a means of solving complex application problems has, in the case of each specific task, its specific features, in particular – in the case when the subject of the study is nanosystems.

The urgency of the work – computer models of nanosystems is easier and more convenient to explore through the simulation and implementation of computing experiments, since real experiments are limited by the physical dimensions of nanosystems and the complexity and speed of processes occurring in nanomaterials.