Abstract

Machine learning and artificial intelligence algorithms have been used to describe and predict the properties of low-dimensional nanostructures. The process of building predictive models based on machine learning algorithms has been employed to: (i) one-dimensional systems: boron nanotubes and boron nitride nanotubes and, two (ii)-dimensional MXenes materials. These systems are presently of interest to researchers due to their unique properties and potential application in medicine and pharmacy.

Predictive models for total system energy, cohesion energy and toxicity have been built. Conducting the research required numerous models based on machine learning algorithmshave been employed to the problems presented in the dissertation. Moreover, all available methods of representing the geometry of the crystal systems ave been tested.

During the work, a unique combination of data from the experiment and theoretical data from numerical simulations have been used. Theoretical data come from open databases containing simulation results and from over 8,500 numerical simulations carried out during the dissertation preparation. The obtained results are based on the analysis of the unique data sets using artificial intelligence algorithms. In addition, the developed methodology allows for explaination of the physical processes and broadens the knowledge about the considered systems. The results describing the toxicity mechanism of MXenes materials seem to be particularly novel and important