Crystal structure prediction of nanowires using evolutionary computations

Tomasz Tarkowski, PhD thesis

Abstract: *The work discusses application of a genetic algorithm in the crystal structure prediction problem. Elements of density functional theory, theory of genetic algorithms with its implementation in C++ programming language and results of the genetic algorithm tuning with use of test functions are shown. The presented knowledge was used to perform structural evolutionary computations in case of the monoatomic nanowires composed of boron atoms with an unit cell of up to 8 atoms in size.*

Keywords: *crystal structure prediction, density functional theory, genetic algorithm, scientific libraries, test functions*