BEAR Evolutionary Algorithm Research – the Road Map for a New Crystal Structure Prediction Software

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Crystal structure prediction (CSP) is an interesting field of computational materials science. Advanced CSP techniques involve artificial intelligence (AI) methods to tackle a complex problem of finding the most favorable forms of condensed matter. The evolutionary algorithm (EA) approach combined with density functional theory (DFT) can be successfully used to achieve this goal.

Some implementations of CSP software using the EA/DFT approach exist [1, 2]. The USPEX code for instance showed to be very successful in the prediction of the structure of superhard and partially ionic phase of bulk boron [3]. However, the domain of CSP of nanowires seems to be still less explored.

In this work, we present a currently developed software package called *BEAR Evolutionary Algorithm Research*, which initial aim is solving the problem of finding the most stable form of all-boron and boron related nanowires via the EA/DFT approach. We will show its current status and the road map of development. In particular, we will explain why we have chosen C++ as the main programming language [4] of the project. Moreover, we will show which open source libraries could be helpful in solving the given problem. We will also explain why we have selected the Evolutionary Computation Framework (ECF) library [5] for the EA part of our work. Furthermore, we will explain how we want to enable an easy setup of calculation process via embedding the Lua scripting language interpreter [6] into the program. Last but not least, we will provide examples of recombination and mutation operators that will be implemented in our program.

In future we want to release our software for free as an open source package.

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[2] D. C. Lonie and E. Zurek, *Comp. Phys. Comm.* **182**, 372 (2011).
[3] A. R. Oganov *et al.*, *Nature* **457**, 863 (2009).
[4] The C++ programming language standard, `https://isocpp.org/std/the-standard`.
[5] Evolutionary Computation Framework, `http://ecf.zemris.fer.hr/`.
[6] The Lua programming language, `http://www.lua.org/about.html`.