XtalOpt Version r12: An Open–Source Evolutionary Algorithm for Crystal Structure Prediction

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Abstract

Version 12 of XtalOpt, an evolutionary algorithm for crystal structure prediction, is now available for download from the CPC program library or the XtalOpt website, `http://xtalopt.github.io`. The new version includes: a method for calculating hardness using a machine learning algorithm within AFLOW-ML (Automatic FLOW for Materials Discovery - Machine Learning), the ability to predict hard materials, a generic optimizer (which allows the user to employ many optimizers that were previously not supported), and the ability to generate simulated XRD (X-ray diffraction) patterns.

Keywords: Structure Prediction; Materials Discovery; Evolutionary Algorithm; Genetic Algorithm; Crystal Structures; Superhard Materials; X-Ray Diffraction Pattern.

PROGRAM SUMMARY

Program Title: XtalOpt
Journal Reference:
Catalogue identifier:
Licensing provisions: 3-Clause BSD [1]
Programming language: C++
Computer: PCs, workstations, or clusters
Operating system: Linux, MS Windows, Mac OS X

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Keywords: Structure Prediction; Materials Discovery; Evolutionary Algorithm; Genetic Algorithm; Crystal Structures; Superhard Materials; X-Ray Diffraction Pattern.
Classification: 7.7
External routines/libraries: Qt [2], Qwt [3], Avogadro2 [4, 5] (optional), libssh [6], Open Babel [7, 8] (separate executable), ObjCryst++ [9, 10] (separate executable), AFLOW-ML [11, 12] (through network), and an external program for optimizing the geometries of extended systems.
Subprograms used: pugixml [13], Spglib [14], XtalComp [15], RandSpg [16].
Nature of problem: Computationally predicting stable and/or hard crystal structures given only their stoichiometry.
Solution method: Evolutionary algorithms (EAs), which use ideas from biological evolution, are optimization algorithms whose goal is to find the optimal solution for a problem that has many degrees of freedom. For *a priori* crystal structure prediction (CSP), EAs search to find the lattice parameters and atomic coordinates that, for example, minimize the energy/enthalpy or maximize the hardness. The XtalOpt EA for crystal structure prediction is published under the 3-Clause BSD License, which is an open source license that is officially recognized by the Open Source Initiative [17]. More information is available in the following publications: XtalOpt's original implementation [18], previous version announcements [19, 20, 21, 22], manuscripts detailing the subprograms XtalOpt employs: XtalComp [23] and RandSpg [24], and the XtalOpt website [25].
Reasons for new version: Since the release of XtalOpt version r11 in January 2018, the following changes have been made:

- Added a hardness calculation via AFLOW-ML (Automatic FLOW for Materials Discovery - Machine Learning).
- Added a hardness fitness function, which allows for the prediction of hard structures.
- Added a generic optimizer, which allows the user to employ many previously unsupported optimizers for minimizing the geometry of an extended system.
- Added the ability to generate a simulated XRD (X-Ray Diffraction) pattern.
- Added the ability to use different optimizers and queuing interfaces for each optimization step.
- Implemented various bug fixes.

Summary of revisions: The theoretical hardness of a crystal can now be automatically calculated during an XtalOpt run. The hardness is calculated through a linear relationship with the shear modulus (originally discovered by Teter [26]) as reported by Chen

[27]. The shear modulus is obtained via AFLOW-ML [11, 12], which employs a machine learning model trained with the AFLOW Automatic Elasticity Library (AEL) [28, 29]. As a result, the EA can employ a new fitness function, which attempts to minimize the enthalpy and maximize the hardness of the predicted structures. This facilitates the search for crystals that are both stable and hard. Additionally, a new generic optimizer was added that allows the user to employ optimizers that were previously not supported (ADF BAND [30] and ADF DFTB [31] are examples that we have thoroughly tested). The only caveat is that the rules for the generic optimizer, which are provided in the online tutorial, must be followed. Open Babel [7, 8] is used to read the output of the generic optimizer. Because of the addition of an executable that uses ObjCryst++ [9, 10], a simulated XRD pattern of a crystal can now also be generated during a structure search. Finally, different optimizers and different queuing interfaces can now be used for each optimization step.

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