XtalOpt Version r11: An Open–Source Evolutionary Algorithm for Crystal Structure Prediction

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Abstract

Version 11 of XtalOpt, an evolutionary algorithm for crystal structure prediction, has now been made available for download from the CPC library or the XtalOpt website, `http://xtalopt.github.io`. Whereas the previous versions of XtalOpt were published under the Gnu Public License (GPL), the current version is made available under the 3-Clause BSD License, which is an open source license that is recognized by the Open Source Initiative. Importantly, the new version can be executed via a command line interface (i.e., it does not require the use of a Graphical User Interface). Moreover, the new version is written as a stand-alone program, rather than an extension to Avogadro.

Keywords: Structure Prediction; Evolutionary Algorithm; Genetic Algorithm; Crystal Structures.

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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
Keywords: Structure Prediction; Evolutionary Algorithm; Genetic Algorithm; Crystal

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Structures.
Classification: 7.7
External routines/libraries: Qt [2], Qwt [3], Avogadro2 [4] (optional), libssh [5] and one of: VASP [6], PWSCF [7], GULP [8], CASTEP [9], SIESTA [10]
Subprograms used: Spglib [11], XtalComp [12], RandSpg [13]
Nature of problem: The computational prediction of a stable crystal structure given only its stoichiometry.
Solution method: Evolutionary algorithms (EAs) are optimization algorithms that use features from biological evolution to attempt to find the global minimum solution for a problem that has many degrees of freedom. In the case of *a priori* crystal structure prediction, EAs search for the atomic coordinates that correspond to the most stable regions of a given potential energy landscape. The XtalOpt EA for crystal structure prediction has now been made available under the 3-Clause BSD License, which is an open-source license that is officially recognized by the Open Source Initiative [14]. More information is available in the following publications: XtalOpt's original implementation [15], previous version announcements [16, 17, 18], and also in manuscripts detailing the subprograms XtalOpt employs: XtalComp [19] and RandSpg [20].
Reasons for new version: Since the release of XtalOpt version r10 in August 2017, the following changes have been made:

- Removed dependence on Avogadro and Open Babel, making XtalOpt a stand-alone program rather than an extension.
- Changed the license from GPLv2 to a 3-Clause BSD license.
- Added the optional use of Avogadro2 to render crystals through a remote procedure call (RPC) protocol.
- Added a command-line interface (CLI) to run the program and generate plots.
- Added the ability for the user to define custom minimum inter-atomic distances (IAD) between pairs of atom types.
- Implemented various bug fixes.

Summary of revisions: Dependence on the programs Avogadro and Open Babel has been removed from XtalOpt, so that XtalOpt is now a stand-alone program instead of an extension. This major development has allowed us to change the license from GPLv2 to the more flexible 3-Clause BSD license. To enable users to continue using Avogadro to render molecules, inter-process communication now occurs through a remote procedure call (RPC) protocol in such a way that a user may open Avogadro2 at any time while the program is running in order to render the crystals they select. A command-line interface

(CLI) has also been added so that the user may run the program without the use of the graphical user interface (GUI). Finally, the ability for the user to define minimum interatomic distances between pairs of atom types allows for more control in creating the initial generation of random structures.

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References:

[1] `https://opensource.org/licenses/BSD-3-Clause`

[2] `https://www.qt.io/`

[3] `http://qwt.sourceforge.net/`

[4] `http://www.openchemistry.org/projects/avogadro2/`

[5] `http://www.libssh.org`

[6] `http://www.vasp.at/`

[7] `http://www.quantum-espresso.org`

[8] `http://nanochemistry.curtin.edu.au/gulp/`

[9] `http://www.castep.org`

[10] `http://www.icmab.es/siesta`

[11] `https://atztogo.github.io/spglib/`

[12] `http://xtalopt.openmolecules.net/xtalcomp/xtalcomp.html`

[13] `http://xtalopt.openmolecules.net/randSpg/randSpg.html`

[14] `http://opensource.org/`

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