XtalOpt Version r7: An Open–Source Evolutionary Algorithm for Crystal Structure Prediction

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Abstract

A new version of XtalOpt, a user-friendly GPL-licensed evolutionary algorithm for crystal structure prediction, is available for download from the CPC library or the XtalOpt website, `http://xtalopt.openmolecules.net`. The new version now supports four external geometry optimization codes (VASP, GULP, PWSCF, and CASTEP), as well as three queuing systems: PBS, SGE, SLURM, and "Local". The local queuing system allows the geometry optimizations to be performed on the user's workstation if an external computational cluster is unavailable. Support for the Windows operating system has been added, and a Windows installer is provided. Numerous bugfixes and feature enhancements have been made in the new release as well.

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

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PROGRAM SUMMARY

Program Title: XtalOpt
Journal Reference:
Catalogue identifier:
Licensing provisions: GPL v2.1 or later [1]
Programming language: C++
Computer: PCs, workstations, or clusters
Operating system: Linux, MS Windows

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Keywords: Structure Prediction; Evolutionary Algorithm; Genetic Algorithm; Crystal Structures.
Classification: 7.7
External routines/libraries: Qt [2], Open Babel [3], Avogadro [4], and
one of: VASP [5], PWSCF [6], GULP [7], CASTEP [8]
Subprograms used: spglib [9], libssh [10]
Nature of problem: Predicting the crystal structure of a system from its stoichiometry alone remains a grand challenge in computational materials science, chemistry, and physics.
Solution method: Evolutionary algorithms are stochastic search techniques which use concepts from biological evolution in order to locate the global minimum of a crystalline structure on its potential energy surface. Our evolutionary algorithm, XtalOpt, is freely available for use and collaboration under the GNU Public License. See the original publication on XtalOpt's implementation [11] for more information on the method.
Reasons for new version: Since XtalOpt's initial release in June 2010, support for additional optimizers, queuing systems, and an operating system has been added. XtalOpt can now use VASP, GULP, PWSCF, or CASTEP to perform local geometry optimizations. The queue submission code has been rewritten, and now supports running any of the above codes on ssh-accessible computer clusters that use the Portable Batch System (PBS), Sun Grid Engine (SGE), or SLURM queuing systems for managing the optimization jobs. Alternatively, geometery optimizations may be performed on the user's workstation using the new internal "Local" queuing system if high performance computing resources are unavailable. XtalOpt has been built and tested on the Microsoft Windows operating system (XP or later) in addition to Linux, and a Windows installer is provided. The installer includes a development version of Avogadro that contains expanded crystallography support [12] that is not available in the mainline Avogadro releases.

Other notable new developments include:

- libssh [10] is distributed with the XtalOpt sources and used for communication with the remote clusters, eliminating the previous requirement to set up public-key authentication
- Plotting enthalpy (or energy) vs. structure number in the plot tab will trace out the history of the most stable structure as the search progresses
- A read-only mode has been added to allow inspection of previous searches through the user interface without connecting to a cluster or submitting new jobs
- The tutorial [13] has been rewritten to reflect the changes to the interface and the newly supported codes. Expanded sections on optimizations schemes and save/resume have been added

- The included version of SPGLIB has been updated. An option has been added to set the cartesian tolerance of the spacegroup detection A new option has been added to the Progress table's right-click menu that copies the selected structure's POSCAR formatted representation to the clipboard
- Numerous other small bugfixes / enhancements

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References:

[1] http://www.gnu.org/licenses/gpl.html

[2] http://www.trolltech.com/

[3] http://openbabel.org/

[4] http://avogadro.openmolecules.net

[5] http://cms.mpi.univie.ac.at/vasp

[6] http://www.quantum-espresso.org

[7] https://www.ivec.org/gulp

[8] http://www.castep.org

[9] http://spglib.sourceforge.net

[10] http://www.libssh.org

[11] D. Lonie, E. Zurek, Comp. Phys. Comm. 182 (2011) 372-387, doi://10.1016/j.cpc.2010.07.048

[12] http://davidlonie.blogspot.com/2011/03/new-avogadro-crystallography-extension.html

[13] http://xtalopt.openmolecules.net/globalsearch/docs/tut-xo.html