# XtalOpt Version r10: An Open–Source Evolutionary Algorithm for Crystal Structure Prediction

Patrick Avery[1], Zackary Falls[1], Eva Zurek[1,]

[a]*Department of Chemistry, State University of New York at Buffalo, Buffalo, New York, 14260-3000*

**Abstract**

A new version of XtalOpt, an evolutionary algorithm for crystal structure prediction, is available for download from the CPC library or the XtalOpt website, `http://xtalopt.github.io`. XtalOpt is published under the Gnu Public License (GPL), which is an open source license that is recognized by the Open Source Initiative. The new version incorporates many bug-fixes and new features, as detailed below.

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

*PACS:*61., 61.50.Ah.

**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, Mac OS X
*Keywords:* Structure Prediction; Evolutionary Algorithm; Genetic Algorithm; Crystal Structures.
*Classification:* 7.7
*External routines/libraries:* Qt [2], Open Babel [3], Avogadro [4], libssh [5] and

*Corresponding author.
*E-mail address:* ezurek@buffalo.edu (E. Zurek)

one of: VASP [6], PWSCF [7], GULP [8], CASTEP [9], SIESTA [10] MOPAC [11], ADF [12], GAMESS [13], Gaussian [14]
*Subprograms used:* SPGLIB [15], RANDSPG [16]
*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 (EAs) are stochastic search techniques that use concepts from biological evolution to search for the global minimum (or a good approximation for it) in a multidimensional problem. Applied to *a priori* crystal structure prediction, EAs search to find atomic arrangements that correspond to stable (low energy or enthalpy) regions of the chemical structure's potential energy landscape. The XTALOPT evolutionary algorithm is available for use and collaboration under the GNU Public License, which is an open-source license that is officially recognized by the Open Source Initiative [17]. See the publication on XTALOPT's original implementation [18] and previous version announcements [19, 20], as well as publications on XTALCOMP [21] and RANDOMDOCK [22], for more information on the method.
*Reasons for new version:* Since the release of XTALOPT version r9 in February 2016 various bug-fixes have been made, along with the addition of several new features:

- Implementation of RANDSPG [23], an algorithm that generates random crystals with specific spacegroups. This algorithm can optionally be used to create symmetric structures in the initial random generation.
- Inclusion of variable forumla units within XTALOPT enables the search for cells with multiple numbers of formula units within a single run.
- A molecular-unit generator permits users to create single-center molecules in the unit cell during the initial generation step.

*Summary of revisions:* RANDSPGhas been incorporated into XTALOPTto allow users to define spacegroups for the initial structure generation. Variable formula units has also been included in order to reduce many runs with various formula units, down to a single run involving a range of formula units. To create molecular-like structures during the initial generation, a molecular-unit builder has been introduced in the version of XTALOPT. **Acknowledgements:** We acknowledge the NSF (DMR-1505817) and the ONR (N000141612583) for financial support and the Center for Computational Research (CCR) at SUNY Buffalo for computational support. This research was supported in part by the New York State Center of Excellence in Materials Informatics.

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