The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction

Eva Zurek
Department of Chemistry, State University of New York at Buffalo, Buffalo, New York, USA
ezurek@buffalo.edu

The past decade has witnessed tremendous advances in first principles calculations, speed-ups in computer hardware, and improvements in algorithms for a priori crystal structure prediction (CSP). These developments have made it possible to predict, without any experimental information, the structure of a crystal given only its composition, opening the door to a new era where materials can be designed rationally prior to their experimental synthesis.

In this contribution we outline some of the methods that have been developed for finding the global minimum structure, and important local minima without experimental information. Focus is placed on describing the XtalOpt evolutionary algorithm (EA) designed in our group towards this end [1-3]. XtalOpt is published under open-source licenses, and the EA searches can be analyzed via the Avogadro chemical editor and visualizer. We describe new algorithmic developments that have made it possible to predict the structures of ever-more complex crystalline lattices. Benchmark tests, which clearly illustrate how the new developments improve the success rate and accelerate the discovery of the global minimum structure, are performed. We describe how XtalOpt has been employed to predict novel ternary hydrides that have the propensity for high-temperature superconductivity under pressure, and superhard materials.

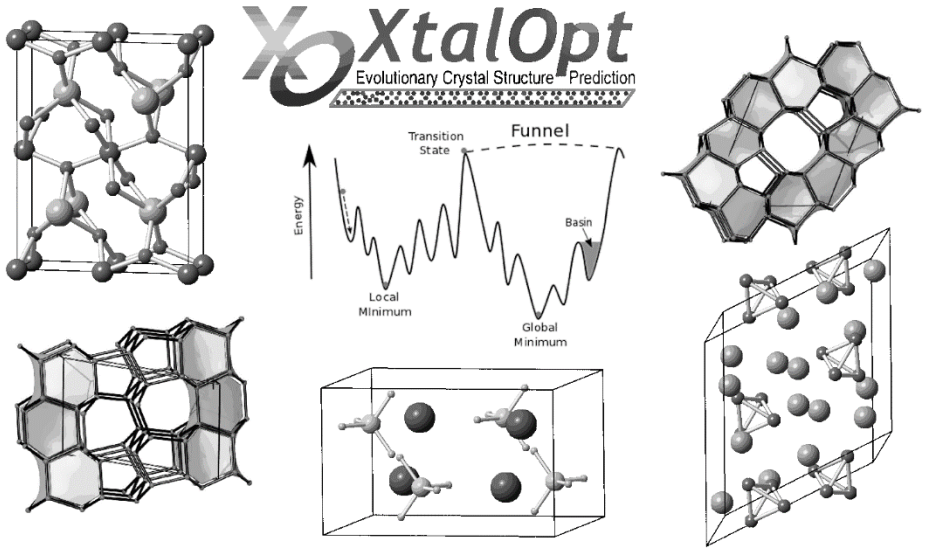

Fig. 1. The XtalOpt evolutionary algorithm for crystal structure prediction can be used to predict the structures of inorganic compounds, including those containing simple molecular units, and superhard materials.

References

[1] Falls Z, Avery P, Wang X, Hilleke KP, Zurek E: The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction, J. Phys. Chem. C. 2021; 125: 1601.
[2] Lonie DC, Zurek E: XtalOpt: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction, Comput. Phys. Commun. 2011; 182: 372.
[3] url: http://xtalopt.github.io/