Predicting the synthesizability and properties of disordered materials by combining first-principles calculations with machine-learning

Cormac Toher[1]
[1]Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, TX 75080, USA

cormac.toher@utdallas.edu

Abstract

The successful development and manufacturing of new materials, for applications ranging from batteries, catalysts and electronics to thermal protection barriers in aerospace engineering, requires extending computational approaches beyond those required for ordered materials to incorporate the effects of disorder and entropy [1-3]. Descriptors and thermodynamic models have been developed to predict the synthesizability and properties of disordered materials [4-6] based on large ensembles of calculations for ordered structures generated using the AFLOW framework for computational materials design [7]. AFLOW automates first-principles calculations: it incorporates a large library of structural prototypes [8-10] that can be decorated with different elements to generate the required input files; it monitors calculations in progress and performs automated error-correction and restart when it detects problems; and it contains modules to calculate thermal and mechanical materials properties [11-13], and to perform thermodynamic stability analysis [14]. AFLOW automatically parses and extracts the relevant data from the output files of completed calculations, which are then made available through the aflow.org data repository [15] and its associated APIs [16]. AFLOW data is being used to predict the synthesizability of new disordered materials such as metallic glasses [17] and high entropy alloys [4], and descriptors have guided the development of new high-entropy carbides [6, 18]. AFLOW data is also being used to train machine-learning models [19], which are available through the aflow.org website. Thermodynamic models are now being combined with machine-learning to predict synthesizability and identify design rules for thermo-mechanical properties [20] for high-entropy silicates, which have applications as thermal and environmental barrier coatings for creep-resistant silicon carbide turbine blades in gas turbine engines, to enable higher operating temperatures leading to increased performance and fuel efficiency.

Figures

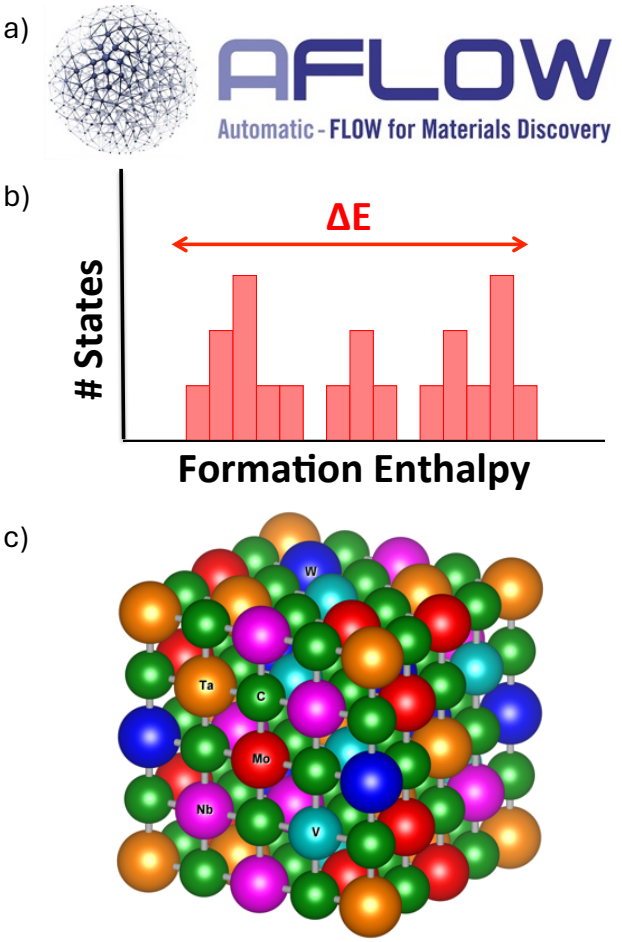

Figure 1. (a) AFLOW uses (b) the distribution of energies of an ensemble of ordered structures to predict the formation and properties of (c) disordered materials.

References

[1] C. Toher, C. Oses, D. Hicks, S. Curtarolo, npj Comput. Mater. **5** (2019) 69.
[2] C. Oses, C. Toher, S. Curtarolo, Nature Rev. Mater. **5** (2020) 295-309.
[3] C. Toher, C. Oses, M. Esters, D. Hicks, G. N. Kotsonis, C. M. Rost, D. W. Brenner, J.-P. Maria, S. Curtarolo, High-entropy ceramics: propelling applications through disorder, MRS Bull. **47** (2022) 194-202.
[4] Y. Lederer, C. Toher, K. S. Vecchio, S. Curtarolo, Acta Mater. **159** (2018) 364–383.
[5] K. Yang, C. Oses, and S. Curtarolo, Chem. Mater. **28** (2016) 6484-6492.
[6] P. Sarker, T. Harrington, C. Toher, C. Oses, M. Samiee, J.-P. Maria, D. W. Brenner, K. S. Vecchio, S. Curtarolo, Nat. Commun. **9** (2018) 4980.
[7] C. Oses, M. Esters, D. Hicks, S. Divilov, H. Eckert, R. Friedrich, M. J. Mehl, A. Smolyanyuk, X. Campilongo, A. van de Walle, J. Schroers, A. G. Kusne, I. Takeuchi, E. Zurek, M. Buongiorno Nardelli, M. Fornari, Y. Lederer, O. Levy, C. Toher, S. Curtarolo, Comput. Mater. Sci. **217** (2023) 111889.

[8] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, S. Curtarolo, Comput. Mater. Sci. **136** (2017) S1–S828.
[9] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, S. Curtarolo, Comput. Mater. Sci. **161** (2019) S1–S1011.
[10] D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, S. Curtarolo, Comput. Mater. Sci. **199** (2021) 110450.
[11] C. Toher, J. J. Plata, O. Levy, M. de Jong, M. Asta, M. Buongiorno Nardelli, S. Curtarolo, Phys. Rev. B **90** (2014) 174107.
[12] C. Toher, C. Oses, J. J. Plata, D. Hicks, F. Rose, O. Levy, M. de Jong, M. Asta, M. Fornari, M. Buongiorno Nardelli, S. Curtarolo, Phys. Rev. Mater. **1** (2017) 015401.
[13] M. Esters, C. Oses, D. Hicks, M. J. Mehl, M. Jahnátek, M. D. Hossain, J.-P. Maria, D. W. Brenner, C. Toher, S. Curtarolo, Nat. Commun. **12** (2021) 5747.
[14] C. Oses, E. Gossett, D. Hicks, F. Rose, M. J. Mehl, E. Perim, I. Takeuchi, S. Sanvito, M. Scheffler, Y. Lederer, O. Levy, C. Toher, S. Curtarolo, J. Chem. Inf. Model. **58** (2018) 2477–2490.
[15] M Esters, C. Oses, S. Divilov, H. Eckert, R. Friedrich, D. Hicks, M. J. Mehl, F. Rose, A. Smolyanyuk, A. Calzolari, X. Campilongo, C. Toher, S. Curtarolo, Comput. Mater. Sci. **216** (2023) 111808.
[16] F. Rose, C. Toher, E. Gossett, C. Oses, M. Buongiorno Nardelli, M. Fornari, S. Curtarolo, Comput. Mater. Sci. **137** (2017) 362–370.
[17] E. Perim, D. Lee, Y. Liu, C. Toher, P. Gong, Y. Li, W. N. Simmons, O. Levy, J. J. Vlassak, J. Schroers, S. Curtarolo, Nat. Commun. **7** (2016) 12315.
[18] S. Divilov, H. Eckert, D. Hicks, C. Oses, C. Toher, R. Friedrich, M. Esters, M. J. Mehl, A. C. Zettel, Y. Lederer, E. Zurek, J.-P. Maria, D. W. Brenner, X. Campilongo, S. Filipović, W. G. Fahrenholtz, C. J. Ryan, C. M. DeSalle, R. J. Crealese, D. E. Wolfe, A. Calzolari, S. Curtarolo, Nature **625** (2024), 66–73.
[19] O. Isayev, C. Oses, C. Toher, E. Gossett, S. Curtarolo, A. Tropsha, Nat. Commun. **8** (2017) 15679.
[20] C. Toher, M. J. Ridley, K. Q. Tomko, D. H. Olson, S. Curtarolo, P. E. Hopkins, E. J. Opila, Materialia **28** (2023) 101729.