FIRST PRINCIPLES COMPUTATIONAL DESCRIPTOR FOR ENTROPY FORMING ABILITY

Stefano Curtarolo, Duke University
stefano.curtarolo@duke.edu
Pranab Sarker, Duke University
Cormac Toher, Duke University
Tyler J. Harrington, University of California, San Diego
Jon-Paul Maria, North Carolina State University
Kenneth S. Vecchio, University of California, San Diego
Donald Brenner, North Carolina State University

Key Words: Entropy, AFLOW, density functional theory

Entropy stabilized materials [1], where the mixing of the components is driven by configurational entropy rather than formation enthalpy, are potential candidates for ultra-high temperature applications. The prediction of which compositions will form entropy stabilized materials is difficult since calculating the entropic contribution to the free energy from first principles is computationally expensive. Therefore, we have formulated a descriptor for the synthesizability of disordered materials based on the energy distribution of the thermodynamic density of states (TDOS) for an ensemble of ordered configurations generated using the AFLOW (Automatic FLOW) partial occupation (AFLOW-POCC) methodology [2,3] and calculated with DFT. This descriptor has been used to successfully predict which refractory metal carbide compositions can be experimentally synthesized as single-phase entropy stabilized materials [4].

This work is supported by the U.S. Office of Naval Research MURI program (grant No. N00014-15- 1-2863).

[1] C. M. Rost, E. Sachet, T. Borman, A. Moballegh, E. C. Dickey, D. Hou, J. L. Jones, S. Curtarolo, and J.-P. Maria, Entropy Stabilized Oxides, Nat. Commun. **6**, 8485 (2015).
[2] S. Curtarolo, W. Setyawan, G. L. W. Hart, M. Jahnatek, R. V. Chepulskii, R. H. Taylor, S. Wang, J. Xue, K. Yang, O. Levy, M. J. Mehl, H. T. Stokes, D. O. Demchenko, and D. Morgan, AFLOW: an automatic framework for high-throughput materials discovery, Comput. Mater. Sci. **58**, 218-226 (2012).
[3] K. Yang, C. Oses, and S. Curtarolo, Modeling off-stoichiometry materials with a high-throughput *ab-initio* approach, Chem. Mater. **28**, 6484-6492 (2016).
[4] P. Sarker, T. Harrington, C. Toher, K. Vecchio, and S. Curtarolo, First principles materials design using a spectral descriptor for entropy forming ability, in preparation (2017).