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Formulation of an entropy descriptor for entropy stabilized compounds from high-throughput DFT PRANAB SARKER, CORMAC TOHER, Dept. of Mech. Eng. and Mat. Science, Duke University, TYLER HARRINGTON, JOSHUA GILD, JIAN LUO, Dept. of NanoEng., UCSD, JON-PAUL MARIA, DON BRENNER, Dept. of Mat. Science and Eng., NCSU, KENNETH VECCHIO, Dept. of NanoEng., UCSD, STEFANO CURTAROLO, Dept. of Mech. Eng. and Mat. Science, Duke University — Entropy stabilized compounds such as entropy stabilized borides, carbides, and oxides [C. M. Rost, *et al.*, Nat. Commun. **6**, 8485 (2015)] are an emerging class of materials in the family of chemically disordered high entropy alloys (HEAs), that are highly attractive candidates for ultra-high temperature applications. The prediction of the synthesizability of these materials using *ab initio* calculations requires the formulation of a descriptor for the existence of a disordered phase at elevated temperature based only on calculations of ordered phases at $T = 0K$. Our proposed descriptor is based on the energy distribution of an appropriate ensemble of different ordered configurations, obtained using Density Functional Theory (DFT) and the AFLOW computational materials design framework. This entropy descriptor can predict the propensity of the composition to form an entropy stabilized single-phase material and shows excellent agreement with the experimental results.

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