FIRST-PRINCIPLES DESIGN AND DISCOVERY OF NEW HIGH-ENTROPY MATERIALS

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High-entropy materials (HEMs) are innovative alloys with five or more principal elements and often exhibit unusual functional properties. These materials are of growing interest, but the design and discovery of HEM design faces daunting challenges. There exists no model capable of robustly predicting which combinations of elements will form a single-phase HEM. In this work [1], we propose a new physical descriptor, based on both enthalpy and entropy considerations, that can enable robust high-throughput screening for new HEMs over large chemical spaces. This descriptor can be easily and quickly calculated from first principles, requiring no experimental or empirically derived inputs. Taking metal carbides as the benchmark system, this descriptor successfully identifies all experimentally reported single-phase high-entropy metal carbides. By this descriptor, these high-entropy carbides are not only clearly separated from those element combinations that are experimentally known to form multiple phases, but also predicted with correct relative magnitudes of their growth temperatures. With this descriptor, tens of new four- and six-metal carbide materials and tens of new 2D high entropy transition metal dichalcogenides are also predicted, and the predicted top candidates also perfectly agree with available experimental results. These newly predicted high entropy materials when synthesized will have the potential for a wide variety of applications such as coating in aerospace devices, energy conversion and storage, and flexible electronics. This work is supported by the U.S. DOE BES.

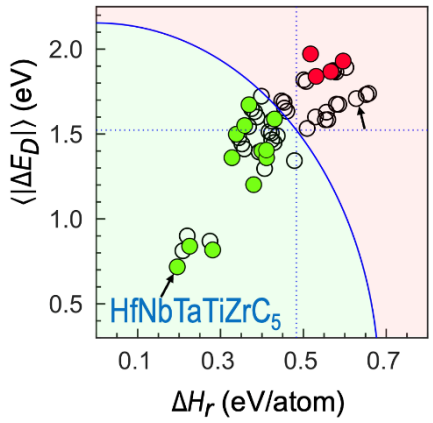

Figure 1 – Descriptor-enabled first principles predictions of high entropy meta carbides. Green: experimentally known single phase high-entropy metal carbides. Red: experimentally attempted element combinations that form multiphase compounds. The closer to the left bottom corner, the higher the synthesizability by prediction.

[1] D. Dey, L. Liang, and L. Yu, "Descriptor-Enabled Rational Design of High-Entropy Materials Over Vast Chemical Spaces," arXiv:2301.06554