Materials synthesizability

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Abstract: One of the great challenges in materials science is the synthesis of the new materials predicted by very/(overly)-optimistic theoretical quantum modeling. The culprit is never in the thermodynamic stability but, instead, in the kinetic of formation of the final product [1]. In this presentation, we see how the statistical analysis of our quantum-data repository (aflow.org) uncovers potential entropy descriptors in the search for effective manufacturability. By leveraging a thermodynamic paradox (samarium-hexaboride nucleation [2]), we analyze the recently discovered family of entropy stabilized oxides [3] (including high-entropy carbides, borides and carbo-borides for super-high temperature materials [4]), and the glass forming ability of metallic glasses [5]. If time and audience's patience allow, we will introduce some recent Machine Learning results dealing with vibrational free energies [6] and energetics/elasticity of materials [7].

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[1] Nat. Mater. 12, 191 (2013); Nat. Mater. 11, 614 (2012);
[2] Appl. Phys. Lett. 105, 222403 (2014);
[3] Nat. Comms. 6, 8485 (2015);
[4] Sarker et al, "Super high-temperature materials design using first- principles spectral descriptors for entropy forming ability" submitted (2017).
[5] Nat. Comms. 7, 12315 (2016);
[6] Chem. Mater. (2017) 10.1021/acs.chemmater.7b00789.
[7] Nat. Comms. 8, 15679 (2017).