Abstract Submitted
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The Thermodynamic Scale of Inorganic Crystalline Metastability[1] WENHAO SUN, STEPHEN DACEK, MIT, SHYUE PING ONG, UCSD, GEOFFROY HAUTIER, UC Louvain, ANUBHAV JAIN, LBNL, WILLIAM RICHARDS, MIT, ANTHONY GAMST, UCSD, KRISTIN PERSSON, GERBRAND CEDER, LBNL, MATERIALS PROJECT TEAM — The space of metastable materials offers promising new design opportunities for next-generation technological materials such as complex oxides, semiconductors, pharmaceuticals, steels and beyond. Although metastable phases are ubiquitous in both nature and technology, only a heuristic understanding of their underlying thermodynamics exists. Here we report a large-scale data-mining study of the Materials Project, a high-throughput database of DFT-calculated energetics of ICSD structures, to explicitly quantify the thermodynamic scale of metastability for 29,902 observed inorganic crystalline phases. We reveal the influence of chemistry and composition on the accessible thermodynamic range of crystalline metastability for polymorphic and phase-separating compounds, yielding new physical insights that can guide the design of novel metastable materials. We further assert that not all low-energy metastable compounds can necessarily be synthesized, and propose a principle of "remnant metastability" – that observable metastable crystalline phases are generally remnants of thermodynamic conditions where they were once the lowest free-energy phase.

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