Prediction of Thermodynamic Stability in Hybrid Organic-Inorganic Elpasolites

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Hybrid organic-inorganic perovskite materials have excellent photovoltaic properties and are inexpensive to synthesize, providing a promising route towards meeting the ever-growing energy demand of the world. Using density functional theory, we explore the thermodynamic stability of hybrid organic-inorganic "double" perovskite structures [$(CH_3NH_3)_2ABiX_6$, A=monovalent cation, X=halide anion] to identify new lead-free materials. We show how combinatorial chemical substitution of existing perovskite-like materials in online materials databases leads to better-populated phase diagrams and improved formation energies using energy vs. composition convex hulls. Finally, we will discuss the use of machine learning to understand relationships between thermodynamic stability and composition-dependent attributes, such as electronegativity and ionic radii.