Ternary and Quaternary Rare-Earth Germanides: Discovery of Intermetallic Compounds from Traditional to Machine-Learning Approaches

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Ternary rare-earth transition-metal germanides \( \text{RE-M-Ge} \) represent a large group of intermetallic compounds that exhibit a rich structural chemistry and many interesting physical properties including superconductivity and magnetocaloric effects. Traditional approaches for materials discovery would involve systematic investigations of phase diagrams, or identification of structural motifs, such as \( \text{MGe} \) ladders and \( \text{Ge}_n \) bridges, to reveal patterns that permit new compounds to be targeted. A different and accelerated approach for materials discovery is through machine-learning techniques, which can be used to predict crystal structures or suggest promising candidates for desired physical properties. We present here case studies of many new ternary (e.g., \( \text{Ce-Rh-Ge} \)) and quaternary (e.g., \( \text{RE}_2\text{M}_2\text{XGe}_4 \) where \( \text{X} = \text{Ag, Cd, In} \)) phases that were discovered through both approaches. In particular, we discuss how machine-learning approaches are valuable in guiding the search for intermetallics that exhibit low thermal conductivity, which is a key criterion for thermoelectric materials.

References