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**Finding the Alloy Genome** GUS L.W. HART, LANCE J. NELSON, Brigham Young University, FEI ZHOU, VIDVUDS OZOLINS, Univ. of California, Los Angeles — First-principles codes can nowadays provide hundreds of high-fidelity enthalpies on thousands of alloy systems with a modest investment of a few tens of millions of CPU hours. But a mere database of enthalpies provides only the starting point for uncovering the “alloy genome.” What one needs to fundamentally change alloy discovery and design are complete searches over candidate structures (not just hundreds of known experimental phases) and models that can be used to simulate both kinetics and thermodynamics. Despite more than a decade of effort by many groups, developing robust models for these simulations is still a human-time-intensive endeavor. Compressive sensing solves this problem in dramatic fashion by automatically extracting the “sparse model” of an alloy in only minutes. This new paradigm to model building has enabled a new framework that will uncover, automatically and in a general way across the periodic table, the important components of such models and reveal the underlying “genome” of alloy physics.

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