Efficient Construction of Robust Materials Models Using Compressive Sensing and Bayesian Inference

LANCE NELSON, GUS L.W. HART, Brigham Young University, FEI ZHOU, VIDVUDS OZOLINS, University of California Los Angeles — Recently, a technique from the field of signal processing, compressive sensing, has emerged as an efficient and robust way to construct models for describing materials’ properties. Compressive sensing exploits the widely-held intuition that the properties of materials can be expressed using a small number of variables. Using this assumption to restrict the solution search results in an efficient way for building very robust models. One way to restrict the model space is through the use of Bayesian inference. In a natural way, Bayesian methods provide error bars on predictions made, a systematic approach for adding data, and noise quantification. We demonstrate Bayesian compressive sensing applied to a cluster expansion model, but the approach is general and could be used in many other model building approaches. This new technique for building materials models, combined with high-throughput ab-initio databases, will allow the fast construction of alloy models for hundreds of systems, representing a major step forward in the endeavor to discover the underlying “genome” of alloy physics.