MM 12: Invited Talk (Hauptvortrag) Hart

Time: Monday 15:00–15:30 Location: BAR 205

Invited Talk MM 12.1 Mon 15:00 BAR 205

Building Thermodynamic Models Made Easy: A Bayesian Compressing Sensing Approach to Automatically Cluster-Expanding 1500 Alloy Systems — •Gus L. W. Hart[1], Lance J. Nelson[1], Conrad W. Rosenbrock[1], Fei Zhou[2], and Vidvuds Ozolins[2] — [1]Dept. of Physics and Astronomy, Brigham Young Univ., Provo UT 84602 USA — [2]Dept of Mat. Sci. and Engineering, University of California, Los Angeles CA 90095 USA

When building physical models (truncated expansions, force-fields, etc.), one often employs the widely-accepted intuition that the physics is determined by a few dominant terms. This reductionist paradigm is limited because the intuition for identifying the those terms often does not exist or is difficult to develop. A "Bayesian compressive sensing" technique provides simple, general, and computationally efficient solution to this challenge. Combined with the high-throughput first principles approach to materials, BCS makes it possible to automatically build models for binary alloy models without human monitoring. Furthermore, the method can automatically adjust to generate the simplest model (fewest terms) that meets a specific accuracy requirement. Beyond the alloy applications, our BCS code can readily be applied to other model building problems. One merely needs a basis representation and training data to build a model in just a few seconds.