Hands-free thermodynamic alloy modeling of 1000 binary alloys using a Bayesian approach

A TALK BY Gus L. W. Hart, Brigham Young University, Utah, USA

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LOCATION	Josef-Stefan-Hörsaal, vormals kleiner Hörsaal der Materialphysik, 3. Stock, Boltzmanngasse 5/Strudelhofgasse 4
ABSTRACT	Bayesian approaches have become useful in recent years as increasing computing power has made them practical. Bayes rule itself is nothing more than a simple statement of conditional probability but can be used to make strong inferences. We discuss the general idea behind Bayes rule and how to use it to build physical models. In the latter part of the talk, I'll talk specifically about a database of about 150,000 first principle calculations, that we are using to build models for nearly 1000 binary alloys *simultaneously* .