Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Structure classification of AB solids via machine learning[1] J.E. GUBERNTIS, G. PILANIA, T. LOOKMAN, Los Alamos National Laboratory — We explored the use of machine learning methods, specifically support vector machines and various forms of cross-validation, for the task of classifying the crystal structures of the octet AB solids. We partitioned a set of 75 solids into rocksalt and non-rocksalt structures and thus performed a binary classification task. We found that using the standard indices (r_σ, r_π), suggested by St. John and Bloch several decades ago, enabled an average success in classification of 92%. Our main new result is our finding that using just r_σ and the excess Born effective charge ΔZ_A of the A atom,computed by DFT, enabled an average success of 98%, prompting us to propose $(r_\sigma, \Delta Z_A)$ as a replacement for the St. John-Bloch pair. In general, we found that adding one or two other features to the St. John-Bloch pair, unless they include the excess Born effective charge, generally decreases the average success rate.

[1]Supported by the Department of Energy.

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Date submitted: 06 Nov 2014 Electronic form version 1.4