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Machine Learning of ABO_3 Crystalline Compounds[1] J. E. GUBERNATIS, P. V. BALACHANDRAN, T. LOOKMAN, Theoretical Division, Los Alamos National Laboratory — We apply two advanced machine learning methods to a database of experimentally known ABO_3 materials to predict the existence of possible new perovskite materials and possible new cubic perovskites. Constructing a list of 625 possible new materials from charge conserving combinations of A and B atoms in known stable ABO_3 materials, we predict about 440 new perovskites. These new perovskites are predicted most likely to occur when the A and B atoms are a lanthanide or actinide, when the A atom is a alkali, alkali earth, or late transition metal, and a when the B atom is a p-block atom. These results are in basic agreement with the recent materials discovery by substitution analysis of Hautier et al. [Inorg. Chem. 50, 656 (2011)] who data-mined the entire ICSD data base to develop the probability that in any crystal structure atom X could be substituted for by atom Y. The results of our analysis has several points of disagreement with a recent high throughput DFT study of ABO_3 crystalline compounds by Emery et al. [Chem. Mat. 28, 5621 (2016)] who predict few, if any, new perovskites whose A and B atoms are both a lanthanide. They also predict far more new cubic perovskites than we do: We predict few, if any, with a high degree of probability.

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