Abstract Submitted
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Invariant Representations for Robust Materials Prediction[1] GUS HART, CONRAD ROSENBROCK, Brigham Young University, GABOR CSANYI, Cambridge University — The high-throughput approach for computational materials science has led to the generation of huge databases of DFT-based calculations. Direct mining of this data has led to the discovery of new materials and is of considerable utility. But the real potential for these data to impact American competitiveness, as envisioned in the MGI, is in "interpolation"—using the data to discover materials not present in the databases. I will discuss an approach for materials interpolation that combines cluster expansion, the new SOAP (smooth overlap of atomic positions) representation, and machine learning.

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