Abstract Submitted
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Invariant Representations of Materials (Or, Making Machine Learning Work)[1] GUS HART, CHANDRAMOULI NYSHADHAM, JACOB E. HANSEN, CONRAD W. ROSENBROCK, ANDREW NGUYEN, Brigham Young University — Efforts to leverage computational materials science to impact meaningful materials discovery are driving rapid growth in materials data. Direct searching of computational databases has already yielded some discoveries. But to really capitalize on the investment and to utilize the full potential of the data, one must be able to effectively explore composition and structure space, a vastly larger space than the space of the data. In other words, we must find a way to effectively interpolate (in composition and structure space) between data points. Recently it has been understood that details of the mathematical representation of materials are key to developing effective algorithms. In simple terms, we discuss the features that a representation must have to be useful for standard data science approaches to be effective.

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