Abstract Submitted for the TSF16 Meeting of The American Physical Society

Discovering materials using machine learning¹ CHANDRAMOULI NYSHADHAM², ANDREW NGUYEN, JACOB HANSEN, GUS L. W. HART, Brigham Young University — Material scientists have developed huge experimental databases of known materials over the last century. Here at BYU we have built a large database of alloy simulations. The challenge now is to develop data-driven methods for designing and discovering new materials. Using such data driven paradigms and extracting the relevant information necessary from the data in a systematic way can be accomplished through an approach known as "machine learning". Machine learning is a subfield of artificial intelligence pertaining to the creation of models that can effectively interpolate from a few known data points. In this talk, I will present a simple understanding of a machine learning model called "scattering transforms" and its usage in discovering new materials. The scattering transform model gives a computer the ability to learn about materials with several elements without being programmed explicitly. This model offers the potential of high accuracy at the speed of machine learning thus accelerating materials discovery.

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²Please put my talk after Dr. Gus Hart's talk in the same session. Thank You.

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