Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Accurate Models of Formation Enthalpy Created using Machine Learning and Voronoi Tessellations LOGAN WARD, ROSANNE LIU, AMAR KRISHNA, VINAY HEGDE, ANKIT AGRAWAL, ALOK CHOUDHARY, CHRIS WOLVERTON, Northwestern Univ — Several groups in the past decade have used high-throughput Density Functional Theory to predict the properties of hundreds of thousands of compounds. These databases provide the unique capability of being able to quickly query the properties of many compounds. Here, we explore how these datasets can also be used to create models that can predict the properties of compounds at rates several orders of magnitude faster than DFT. Our method relies on using Voronoi tessellations to derive attributes that quantitatively characterize the local environment around each atom, which then are used as input to a machine learning model. In this presentation, we will discuss the application of this technique to predicting the formation enthalpy of compounds using data from the Open Quantum Materials Database (OQMD). To date, we have found that this technique can be used to create models that are about twice as accurate as those created using the Coulomb Matrix and Partial Radial Distribution approaches and are equally as fast to evaluate.

Logan Ward
Northwestern Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4