**Controlling Spin Ordering in Rare-Earth Perovskite Vanadates**
NICHOLAS WAGNER, JAMES RONDINELLI, Northwestern University — We
investigate the role and influence of local structure distortions on the antiferromag-
netic spin ordering temperatures for large $A$-site radii $R$VO3 perovskites ($R$=Yb-La)
using a combination of data analytics (DA) and density functional theory (DFT).
First, mode crystallography is used to parameterize the structural phase space. Next,
we identify the important local structural features that correlate strongly with the
Néel temperatures ($T_N$) using Pearson correlation coefficients. From this data, we
then formulate a regression model using gradient boosted decision trees (GBDT)
that returns the relative importance of each feature in predicting $T_N$. Our analy-
sis indicates that the amplitude of the subtle Jahn-Teller active mode, which leads
to variations in the V-O bond lengths and angles, could be used as an effective
structural control parameter to modify the spin ordering temperature. We then
validate this data-driven structure-property relationship in artificial vanadate struc-
tures using $T_N$ based on both our GBDT model and a model Hamiltonian using
DFT energies. This combined approach allows us to gauge the accuracy of existing
physical models for the antiferromagnetic ordering in vanadates and opens possible
strategies to design materials with targeted $T_N$.

Nicholas Wagner
Northwestern University

Date submitted: 04 Nov 2015                    Electronic form version 1.4