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 antiferromagnetic spin ordering temperatures for large A-site radii RVO3 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 analysis 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 structures 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 $T_N$.

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