Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Role of Exchange and Correlation in Predicting Structures and Properties of Fluoride Materials NENIAN CHARLES, Drexel University, JAMES RONDINELLI, Northwestern University — The study of fluorine-based inorganic compounds has captured the attention of condensed matter physicists as a route to engineer novel states of matter. Here, we present a density functional theory (DFT) study on fluorides with structures ranging from simple to complex, including KF (rock salt), MnF_2 and VF_2 (rutile), $KMnF_3$ (perovskite), and Na_3MnF_6 and Na_6ScF_6 (cryolite). The focus is on understanding the accuracy of various exchange-correlation functionals for the prediction of structural, electronic, and phonon properties at four different levels of theory, i.e., the local density approximation (LDA), generalized gradient approximation (GGA), meta-GGA, and hybrid functional level with exact exchange. Specifically, we draw attention to the meta-GGA functional MS2 [Sun *et al*, Phys. Rev. Lett., **111**, 106401 (2013)], demonstrating that although it shows improvements over the LDA and GGA functionals in predicting structural properties of fluorides, MS2 generally performs poorer for the electronic and phonon properties. Our study provides useful insights for predictive design of functional halide compounds using computational models based on DFT.

Nenian Charles
Drexel University

Date submitted: 05 Nov 2015 Electronic form version 1.4