Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Machine learning energies of 2M elpasolite (ABC_2D_6) crystals
FELIX A. FABER, Univ of Basel, ALEXANDER LINDMAA, Linkping University, O. ANATOLE VON LILIENFELD, University of Basel, RICKARD ARMIENTO, Linkping University — Elpasolite is one of the most predominant quaternary crystal structures ($AlNaK_2F_6$ prototype) reported in the Inorganic Crystal Structure Database. We present a machine learning model to calculate density functional theory quality formation energies for all 2M possible ABC_2D_6 elpasolite crystals one can make up from all main-group elements up to Bi. The model's accuracy can be improved systematically, reaching a mean-absolute out of sample error of 0.1 eV/atom after training on 10k crystals. Out of the 2M crystals, we have identified 128 new structures which we predict to be on the convex hull—among which $NFAl_2Ca_6$, a metallic elpasolite with unusual stoichiometry and negative atomic oxidation state of Al.

Felix A. Faber
Univ of Basel

Date submitted: 26 Oct 2016 Electronic form version 1.4