Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Predictive Modeling for Strongly Correlated f-electron Systems: A first-principles and database driven machine learning approach[1] TOWFIQ AHMED, Los Alamos Natl Lab, ADNAN KHAIR, MUEEN ABDULLAH, University of New Mexico, HEIKE HARPER, OLLE ERIKSSON, Uppsala University, JOHN WILLS, JIAN-XIN ZHU, ALEXANDER BALATSKY, Los Alamos National Laboratory — Data driven computational tools are being developed for theoretical understanding of electronic properties in f-electron based materials, e.g., Lanthanides and Actnides compounds. Here we show our preliminary work on Ce compounds. Due to a complex interplay among the hybridization of f-electrons to non-interacting conduction band, spin-orbit coupling, and strong coulomb repulsion of f-electrons, no model or first-principles based theory can fully explain all the structural and functional phases of f-electron systems. Motivated by the large need in predictive modeling of actinide compounds, we adopted a data-driven approach. We found negative correlation between the hybridization and atomic volume. Mutual information between these two features were also investigated. In order to extend our search space with more features and predictability of new compounds, we are currently developing electronic structure database. Our f-electron database will be potentially aided by machine learning (ML) algorithm to extract complex electronic, magnetic and structural properties in f-electron system, and thus, will open up new pathways for predictive capabilities and design principles of complex materials.

[1]NSEC, IMS at LANL

Towfiq Ahmed
Los Alamos Natl Lab

Date submitted: 11 Nov 2016 Electronic form version 1.4