Predictive Modeling for Strongly Correlated *f*-electron Systems:

A first-principles and database driven machine learning approach

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Abstract: We are developing data driven computational tools for theoretical understanding of electronic properties in *f*-electron based materials, e.g., 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 are developing electronic structure database which 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.

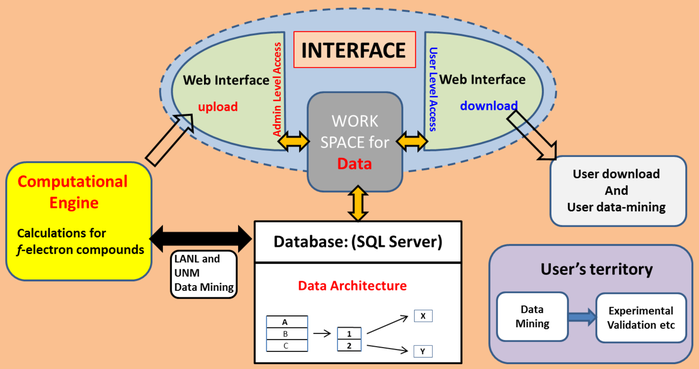
Overview

Goal: Explore the rich and complex electronic and structural properties of *f*-electron systems aided by theory, large simulated data and machine learning (**ML**) methods in order to achieve deeper physical understanding and better predictability to engineer next generation correlated materials.

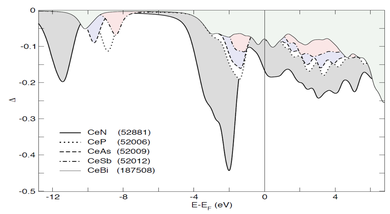
Why "Theory + ML " ?

Theory → Accurate physical theories for strongly correlated system involve quantum many-body effect. Thus, computationally extremely expensive and impractical for simulating larger systems.

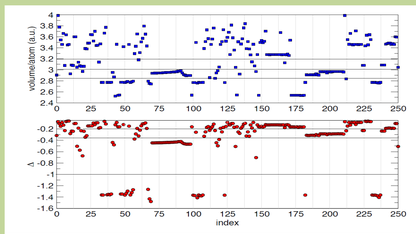
Theory + ML → Density functional theory with LDA gives approximate results and computationally faster. Therefore, aided by large number of simulation data and ML, qualitative trend can help build new physical insight.



Example DFT Calculation: Ce compounds

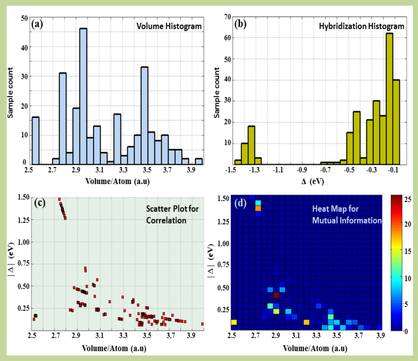


Calculated hybridization function Δ depends on the energy relative to the Fermi level E_F for binary Ce compounds. The numbers in the brackets denote the ICSD references number.



Maximum values of the hybridization function for binary cubic Ce compounds (bottom) and the experimental volume/atom for the same set of compounds (top).

Correlation between 'Volume' and 'Hybridization'



(a) and (b) are the distribution of 257 Ce compound data on volume/atom (V) and hybridization energy (Δ) correspondingly. In (c) Δ vs. V provides correlation between the two data sets (see text for details). 2D heat-map is (d). Colors represents the number count of Ce compounds in each cell. Heat-map provides joint probability distribution and measures mutual information I(V, Δ).

Reference: Manuscript under preparation

(c) Correlation Coefficient:

$$r(V,\Delta) = \frac{\sum_{i=1}^{257}(V(i)-\bar{V})(\Delta(i)-\bar{\Delta})}{\sqrt{(\sum_{i=1}^{257}(V(i)-\bar{V})^2)(\sum_{i=1}^{257}(\Delta(i)-\bar{\Delta})^2)}} = -0.5565$$

(c) Mutual Information:

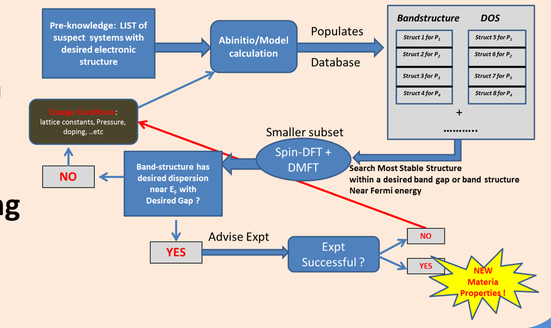
$$I(V,\Delta) = \sum_{i\in V, j\in\Delta} P(i,j)log(\frac{P(i,j)}{P(i)P(j)}) = 0.5757.$$

Database Web Interface for *f*-electron System

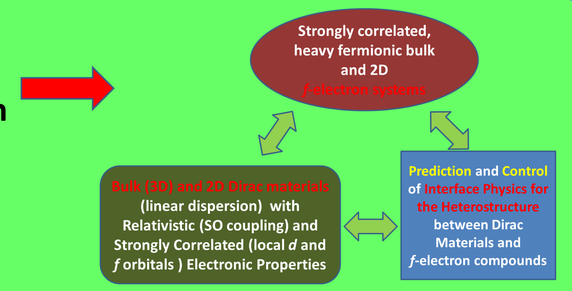
Website Hosted at NMC Server by Institute for Materials Sciences, LANL

Snapshot

Prediction using ML and Datamining



Future Direction



Acknowledgement

This work was supported by Institute for Materials Science at LANL which is a DOE facility under Contract No. DE-AC52-06NA25396 .

LA-UR –16-23417