The Local Spectroscopy Data Infrastructure (LSDI)

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Overview

- The LSDI project aims to establish a unique computational infrastructure for the production, curation, analysis, dissemination and sharing of X-Ray Absorption (XAS) and Nuclear Magnetic Resonance (NMR) spectroscopy data, and correlating such spectra these with specific electronic structure, bonding and local atomic environments.
- The effort leverages the software infrastructure of the Materials Project(MP) to develop a completely integrated, one-stop platform for first principles XAS/NMR data, including experimental benchmarks and comparison tools.
- Develop software infrastructure for the storage and dissemination of experimental data: **MPContribs**.

Computational Spectroscopy

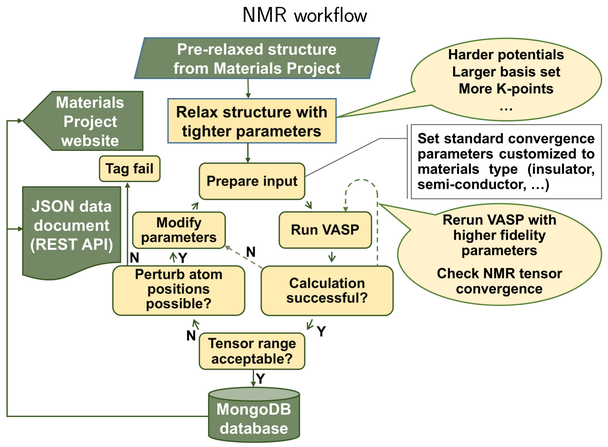
- **NMR Spectra**
  - Yields information on the chemical shift which depends heavily on the local atomic configuration.
  - Computed at the first principles level using the Density Functional Theory(DFT) and linear response theory.
  - Spectra computed using the Vienna Ab-initio Software Package (VASP).
- **XAS Spectra**
  - Measures the absorption of X-rays as a function of the incident beam energy.
  - XAS gives a unique signature of a given material and depends on the detailed atomic structure and electronic and vibrational properties of the material.
  - Multiple-scattering theory used to compute the spectra.
  - FEFF software that implements the green's function based multiple-scattering theory is used to compute the XAS spectra.

High Throughput Workflow infrastructure

- The software infrastructure is built on the open source python packages that power the Materials Project:
  - Structure manipulations/ input set creation / output files processing: Pymatgen
  - Workflow creation and management: Fireworks
  - Workflow recipes package: MatMethods

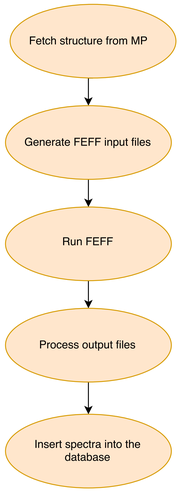
NMR Data Infrastructure: Status Quo

- Fully automated workflow for NMR with the results stored in database for distribution and further analysis.
- Work in progress: proton position sensitive and molecular motion dependent workflows

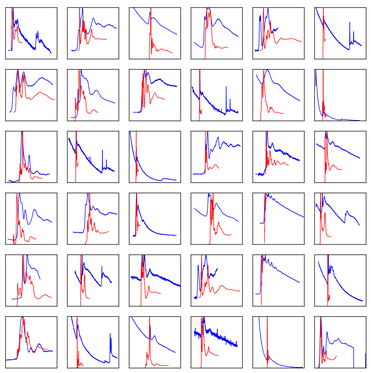


XAS Data Infrastructure: Status Quo

- Developed open source software tools for the high throughput generation and storage of XAS spectra. It is fully functional and rigorously tested.
- Rigorous benchmarking on over 100 experimental spectra.
- Production underway: over 10000 K-edge spectra spanning over 1500 compounds from the Materials Project database so far.
- Work in progress: tuning FEFF parameters for higher edge(L1, L2) spectra calculations.

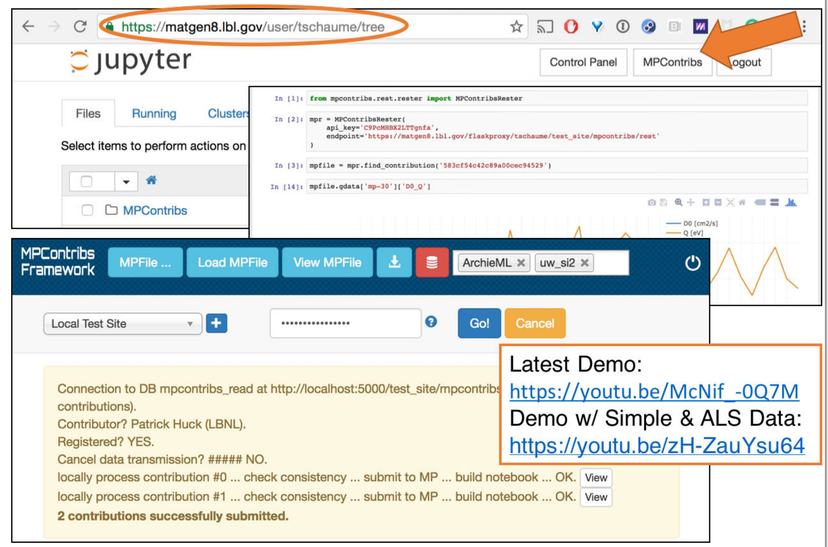


XAS Workflow

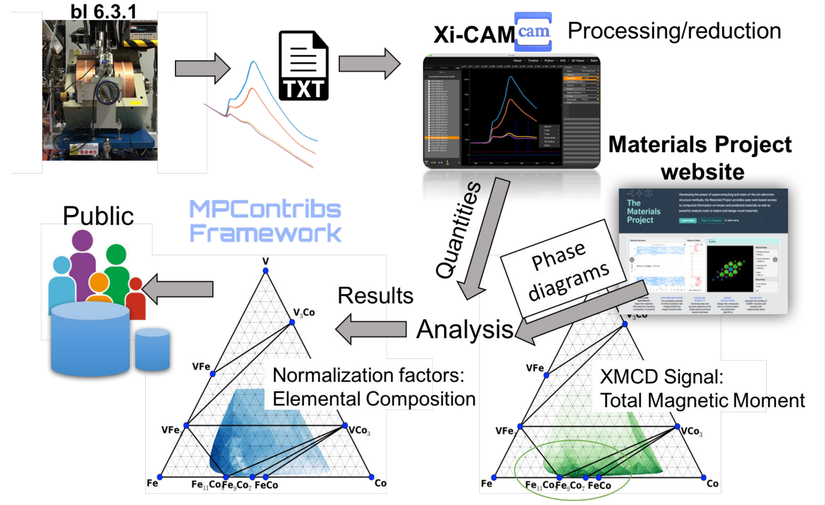


K-edge benchmark: ELNES experimental(blue) vs computed(red)

MPContribs: Public JupyterHub Release



MPContribs: NEXAFS Workflow Integration



Acknowledgements

This material is based on work supported as part of the DIBBS project funded by NSF, under Award Number 1640899. The computational resources were provided by NERSC and SDSC.

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