

Effective and interactive dissemination of diffusion data using MPContribs

Patrick Huck

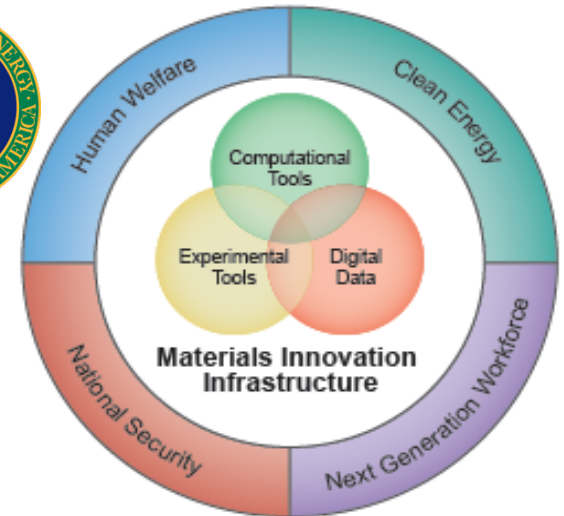
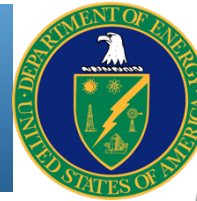
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MGI & Materials Project: Achievements to Date



2011: “make the process of **discovery & development of advanced materials faster, less expensive, more predictable**”

“solutions in most pressing areas require advanced materials”

High-Quality
Materials DATA

- **> 70,000 relaxed compounds:** validated energy, phase diagrams
- **> 70,000 Pourbaix diagrams:** world’s largest set
- **> 43,000 band structures** + higher accuracy 2,700 band gaps
- **> 3,000 elastic tensors:** world’s largest data set


Rapid
DISSEMINATION

- **Ten Apps** enabling material searching and design
- **First Materials data API** ; community download > 8 million data
- **MPContribs framework:** platform for data sharing
- **Over 25,000 registered users !**

DESIGN

Design of **novel functional materials**
(photocatalysts, thermoelectrics, cathodes/electrolytes)

MP Web Site – A Science Gateway

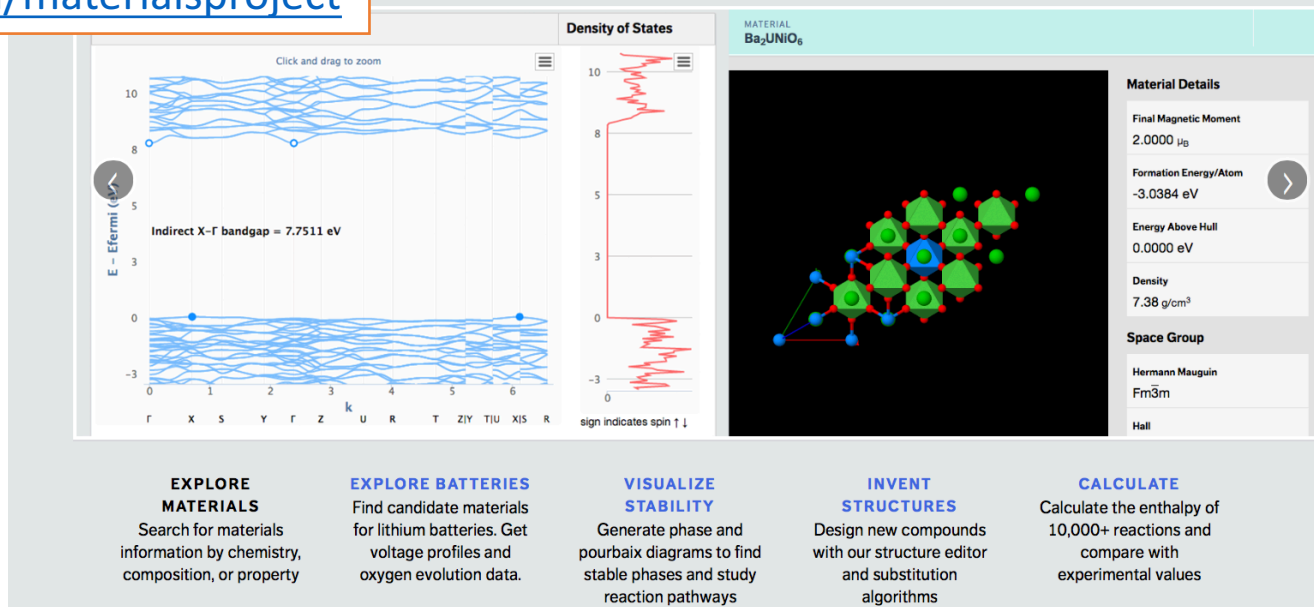


The Materials Project

Harnessing the power of supercomputing and state-of-the-art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Learn more](#) [Sign In or Register](#) to start using

<https://materialsproject.org/>
<https://github.com/materialsproject>



State-of-the-art
OPEN SOURCE
CODES

- **Developed and disseminated key code base:**
- **FireWorks** workflow
- **pymatgen**; comprehensive analysis code
- **Custodian** failure recovery

Contribute data and disseminate it through MP

MPCONTRIBS

“help sharing datasets with the world”

A. T. N'Diaye (ALS, LBNL):

- measured XAS/XMCD spectra
- properties of rare earth substitutes
- processing of instrumental data
- integration w/ MP phase diagrams

D. Morgan, H. Wu (SI2, UW):

- computed diffusion coefficients
- automated VASP data extraction and integration with MP

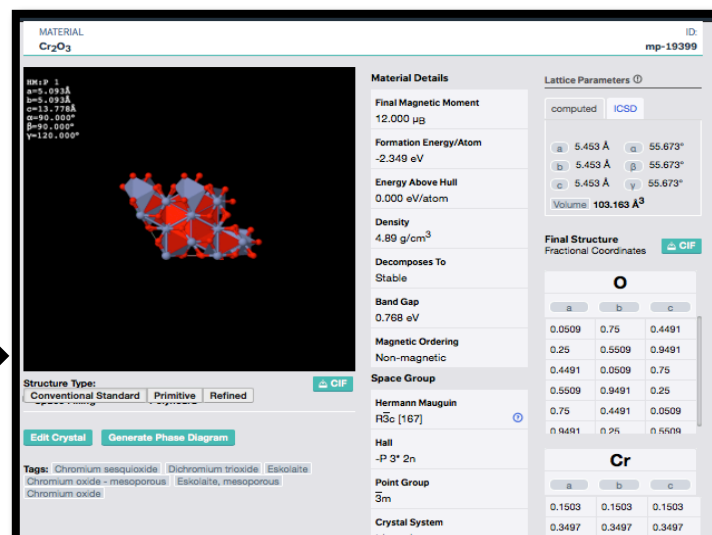
Demo w/ Simple & ALS Data:

<https://youtu.be/zH-ZauYsu64>

Demo of UW/SI2 Web App:

<https://youtu.be/wbWde5StHnU>

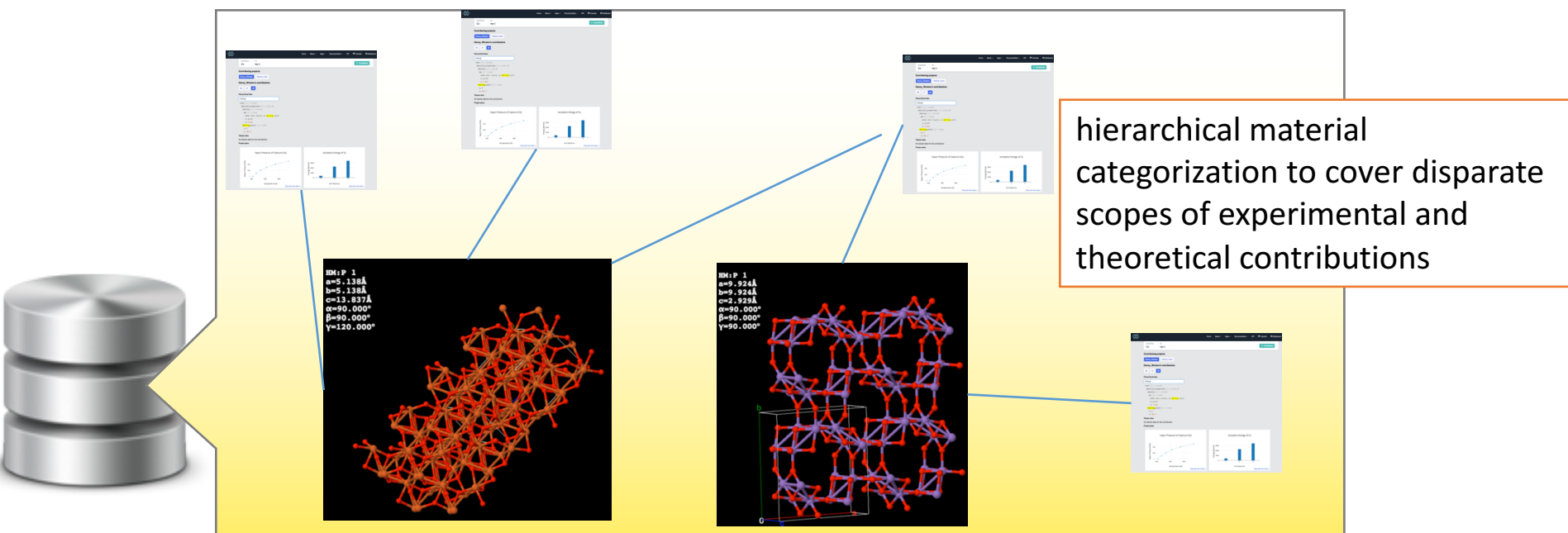
Annotate materials already existing in core database



aim to develop a customized web app driven by MPMCONTRIBS

- Establish a Center Hub for theoretical and experimental data
- Effective dissemination for exposure to large MP user community

Collective Annotation of Core Database



materials/mp-24972/contributions
(mostly theoretical contributions)

links to

compositions/Fe₂O₃/contributions
(experimental contributions)

ternary plot
representation,
e.g. phase diagrams

Symmetry + Lattice

Specific
compositions

multiple
compositions

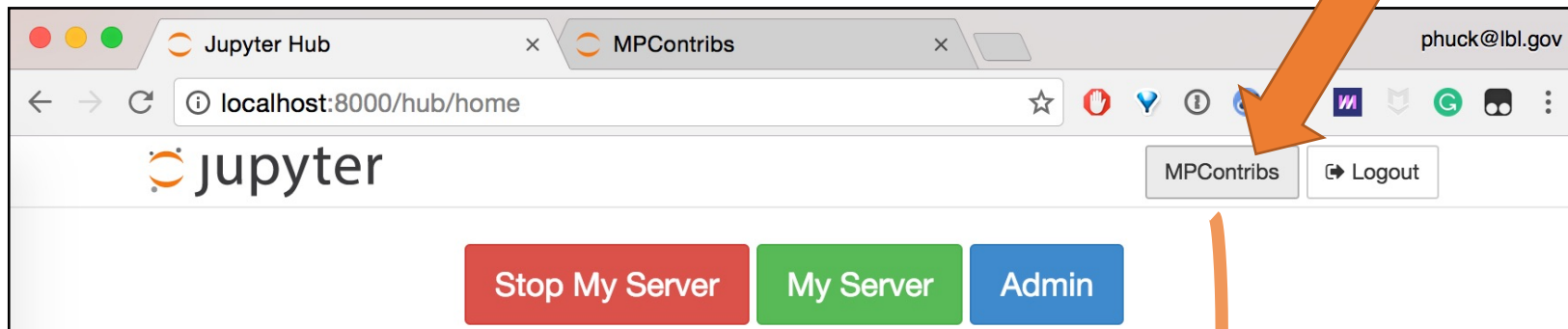
raw user files

experimental instruments
theoretical calculations

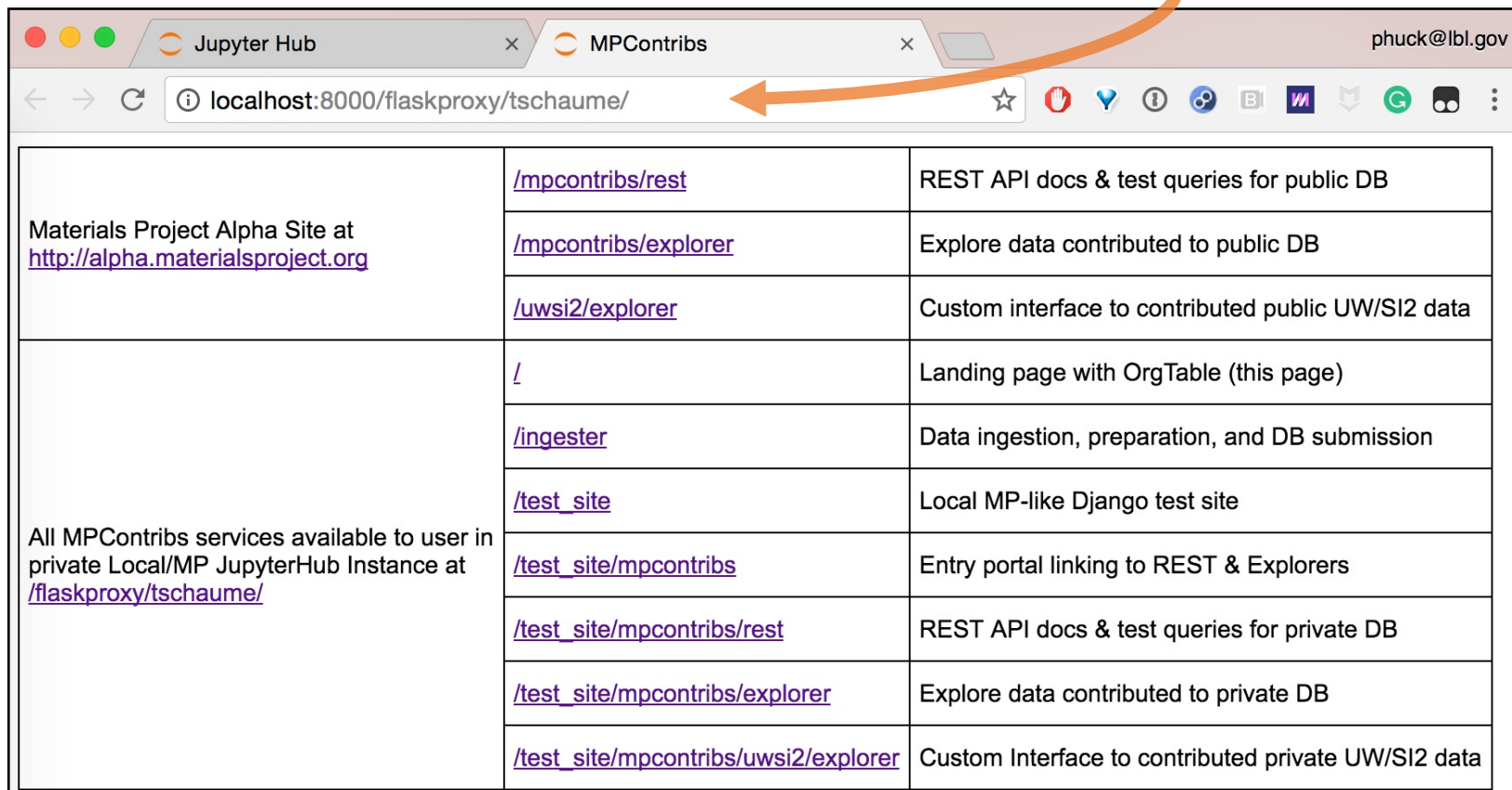
Categories [Identifiers]

Structure [mp-24972]
< Composition [Fe₂O₃]
< Chem. System [Fe*O*]

Integration with JupyterHub



A screenshot of a web browser showing the JupyterHub interface. The browser has two tabs: 'Jupyter Hub' and 'MPContribs'. The address bar shows 'localhost:8000/hub/home'. The page features the Jupyter logo on the left and a 'Logout' button on the right. Below these are three large buttons: 'Stop My Server' (red), 'My Server' (green), and 'Admin' (blue). An orange arrow points from the 'MPContribs' button in the top right to the 'MPContribs' button in the screenshot below.



A screenshot of a web browser showing the MPContribs services page. The browser has two tabs: 'Jupyter Hub' and 'MPContribs'. The address bar shows 'localhost:8000/flaskproxy/tschaume/'. The page contains a table with two columns: 'Materials Project Alpha Site at' and 'All MPContribs services available to user in private Local/MP JupyterHub Instance at'. The table lists various services and their descriptions.

Materials Project Alpha Site at http://alpha.materialsproject.org	/mpcontribs/rest	REST API docs & test queries for public DB
	/mpcontribs/explorer	Explore data contributed to public DB
	/uws2/explorer	Custom interface to contributed public UW/SI2 data
All MPContribs services available to user in private Local/MP JupyterHub Instance at /flaskproxy/tschaume/	/	Landing page with OrgTable (this page)
	/ingerster	Data ingestion, preparation, and DB submission
	/test_site	Local MP-like Django test site
	/test_site/mpcontribs	Entry portal linking to REST & Explorers
	/test_site/mpcontribs/rest	REST API docs & test queries for private DB
	/test_site/mpcontribs/explorer	Explore data contributed to private DB
	/test_site/mpcontribs/uws2/explorer	Custom Interface to contributed private UW/SI2 data

Data Preparation, Ingestion & Submission

The screenshot displays the MPContribs Framework interface, which is used for data preparation, ingestion, and submission. The interface is divided into several sections:

- Top Bar:** Contains the MPContribs Framework logo and navigation buttons: MPFile ..., Load MPFile, View MPFile, and a download icon. It also shows active tabs for ArchieML and uw_si2.
- Left Panel:** Features a search bar and a sidebar with tabs for h-Data, Tables, Graphs, and Inputs. Below these tabs are input fields for Host_lattice_constant_a_angstrom, Host_melting_temperature_K, and Host_vacancy_formation_energy_eV. A plot area shows a blue bar chart with a tooltip displaying coordinates (x: 4.039094, y: 0.4847, z: 933) and material ID (mp-134 b822eda).
- Right Panel:** Contains a code editor with Python code for loading and processing data. The code includes comments like "mission processing of 'uw_si2' project" and "users.uw_si2.pre_submission import run". Below the code is a terminal window showing output: "1546772", "meta-data from figshare", "share into DataFrame", "info, and add additional info", and "124".
- Bottom Panel:** Shows a "Local Test Site" dropdown, a "+" button, and a "Go!" button. Below this is a large yellow box containing the submission status: "Connection to DB mpcontribs_read at http://localhost:5000/test_site/mpcontribs/rest? OK (0 contributions). Contributor? Patrick Huck (LBNL). Registered? YES. Cancel data transmission? ##### NO. locally process contribution #0 ... check consistency ... submit to MP ... build notebook ... OK. View locally process contribution #1 ... check consistency ... submit to MP ... build notebook ... OK. View 2 contributions successfully submitted."

Explorer & REST Interfaces

[Home](#)[Dashboard](#)[Logout](#)

Explore contributed **Materials** or **Compositions** ?

Select (one or more) materials and/or projects:

Or enter a (list of) contribution identifiers:

Result
/test_
/test_

```
In [26]: from mpcontribs.rest.rester import MPContribsRester
```

```
In [27]: SITE = 'http://localhost:5000/test_site' # or http://alpha.materialsproject.org
API_KEY = 'Gn6tOpaHM1EAsbTr' # copy from SITE dashboard
ENDPOINT = SITE + '/mpcontribs/rest' # REST API endpoint for SITE
mpr = MPContribsRester(API_KEY, endpoint=ENDPOINT)
```

```
In [28]: # make sure that user is registered on SITE as contributor
assert(mpr.check_contributor()['is_contrib'])
contribs = mpr.query_contributions() # get list of user contributions
cid = contribs[0]['_id'] # contribution identifier (ObjectId)
```

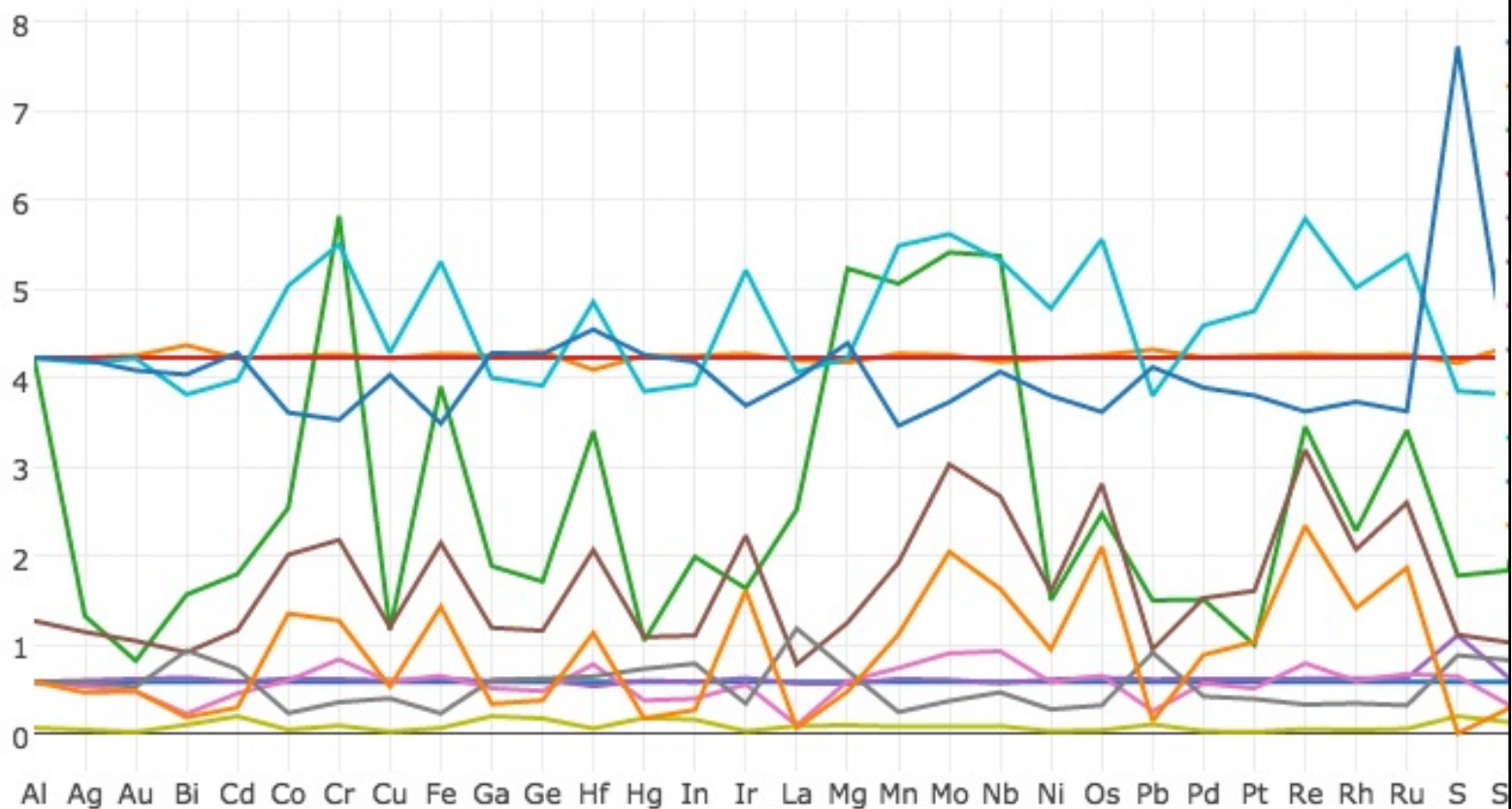
```
In [29]: mpfile = mpr.find_contribution(cid) # get MPFile object from MPContribsRester
mpid = mpfile.ids[0] # MP material identifier (e.g. mp-134)
```

MPFile Components

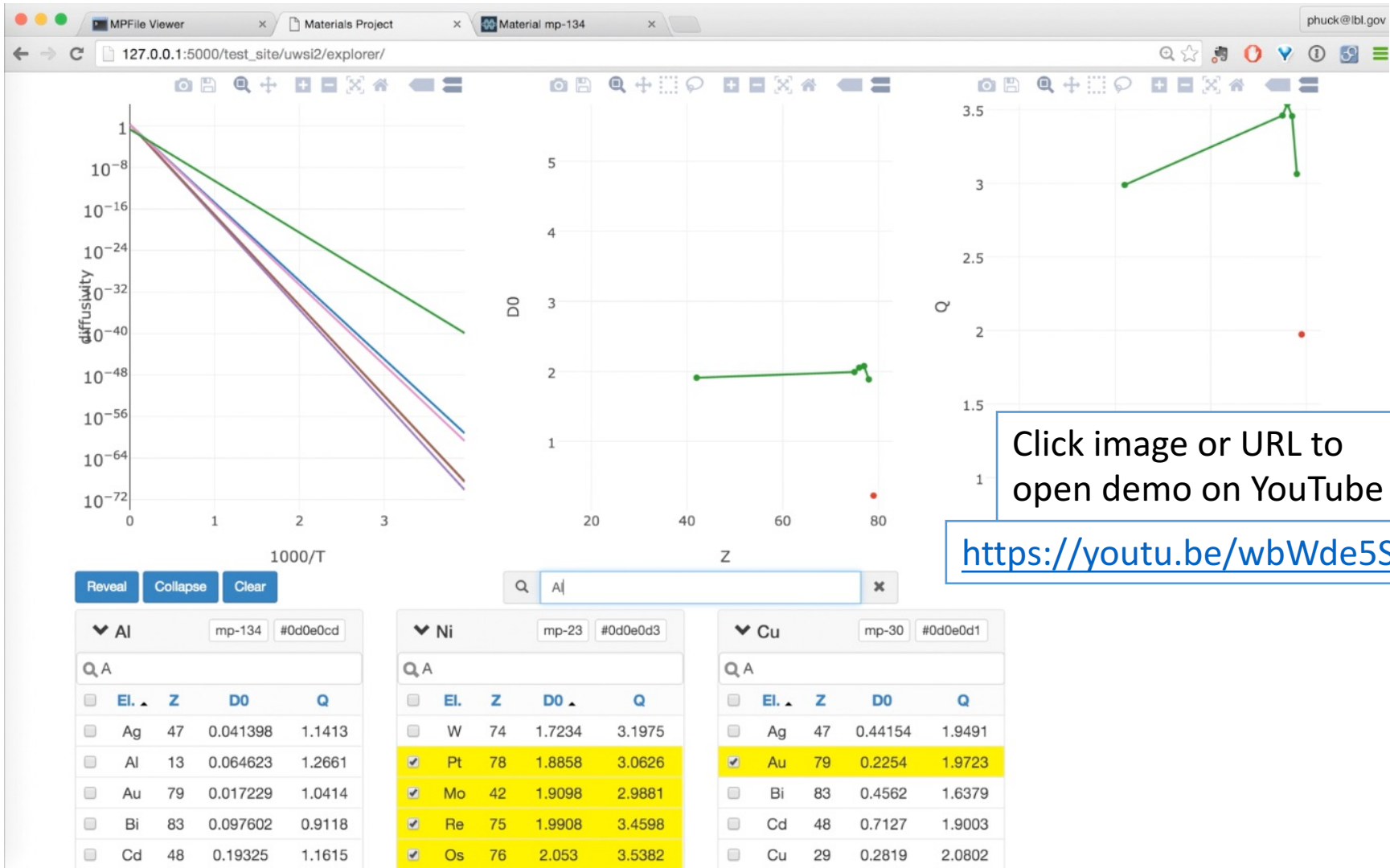
```
In [30]: mpfile.hdata[mpid] # show hierarchical data contained in MPFile for mp-134
```

```
In [31]: mpfile.tdata[mpid]['data_supporting'] # show a specific table contained in MPFile
```

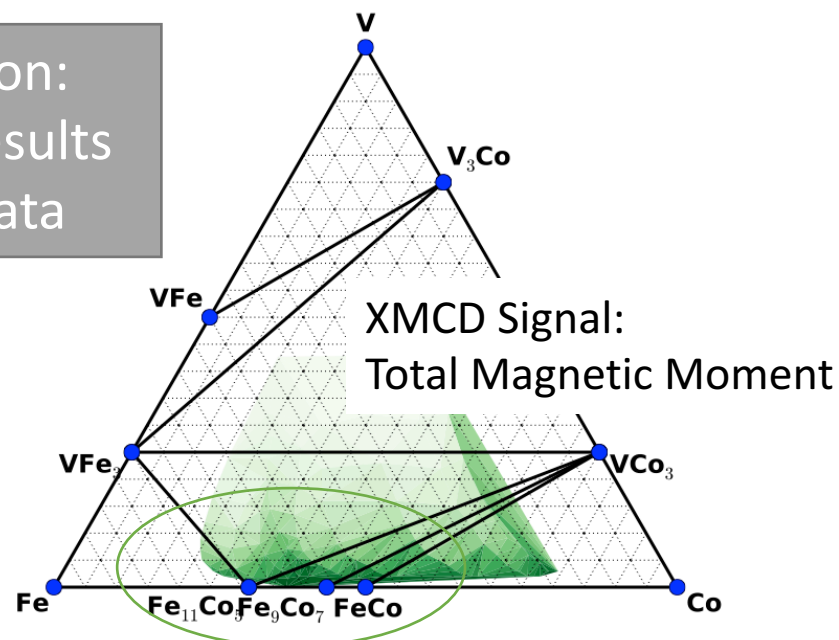
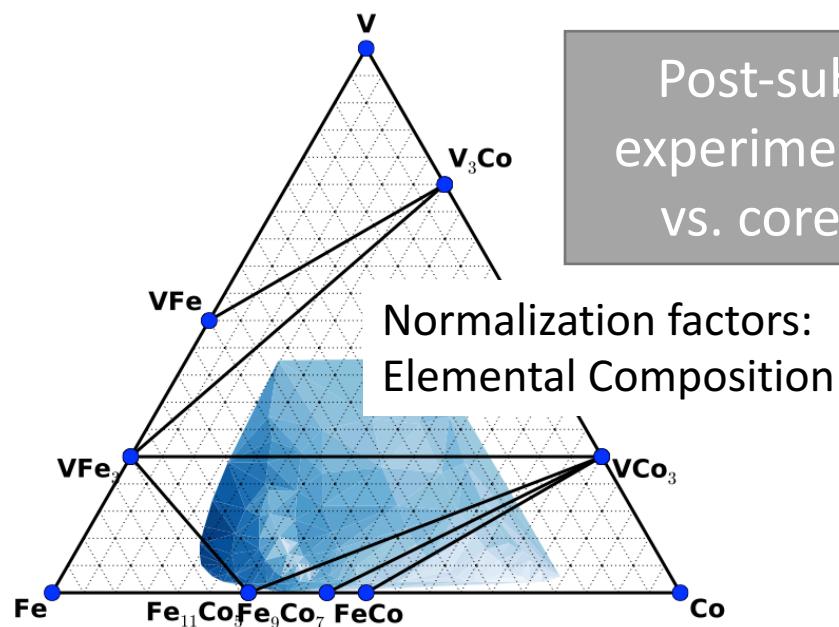
```
In [32]: mpfile.gdata[mpid]['supporting'] # show graphs for specific table contained in MPFile
```



UW/SI2 Diffusion App - Demo



XMCD/Magnetic Moment \leftrightarrow PD



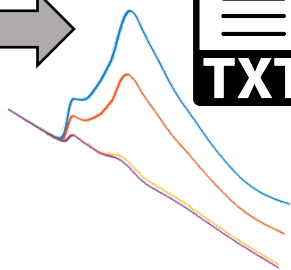
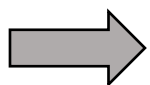
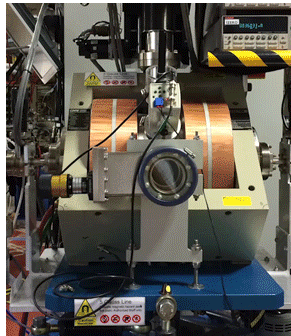
Does data coincide w/ any phase transitions or stable compounds?

MPCONTRIBS helps the Collaborator:

1. guide the planning of (follow-up) computations and experiments
2. understand results of unknown materials
3. provide reference of well understood materials
4. reduce manual repetitive analysis work

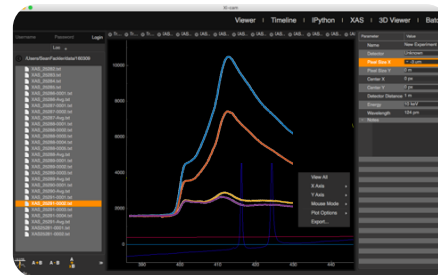
The High-throughput NEXAFS workflow

bl 6.3.1

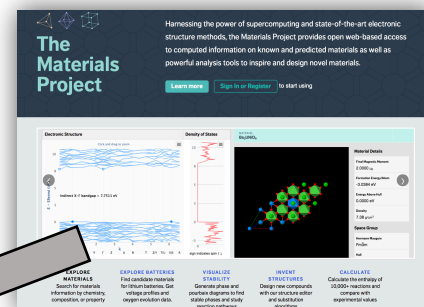


Xi-CAM 

Processing/reduction



Materials Project
website

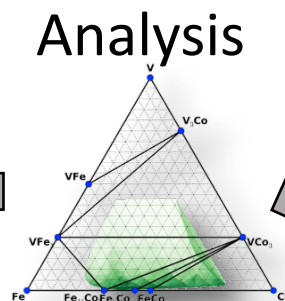


Quantities



Analysis

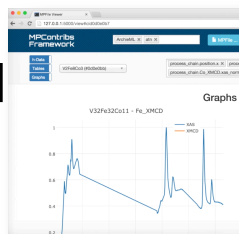
Phase
diagrams



Result



MPContribs
Framework



Public

