

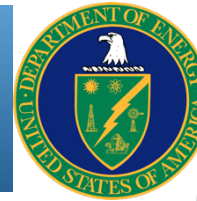
Infrastructure to enable user contributions to Materials Project

# **MPCOMPLETE & MPCONTRIBS**

# MGI & Materials Project: Achievements to Date

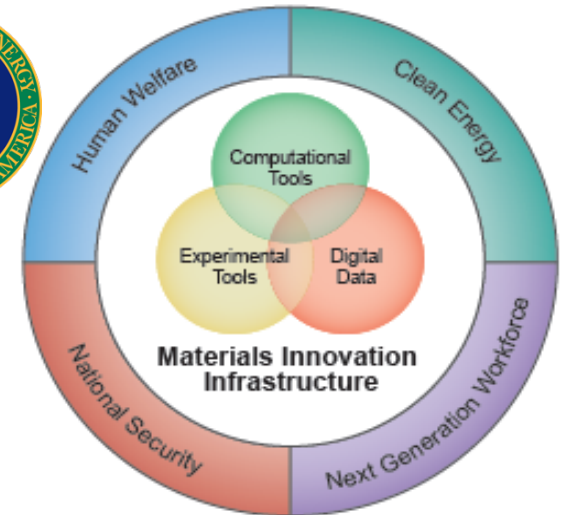


## Materials Genome Initiative



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

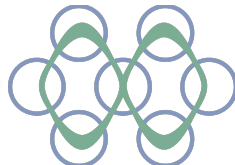
- > **60,000 relaxed compounds**: validated energy, phase diagrams
- > **70,000 Pourbaix diagrams**: world's largest set
- > **28,000 band structures** + higher accuracy 2,700 band gaps
- > **1,300 elastic tensors**: world's largest data set

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 14,000 registered users !**

DESIGN

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



# MP Web Site – A Science Gateway



## The Materials Project

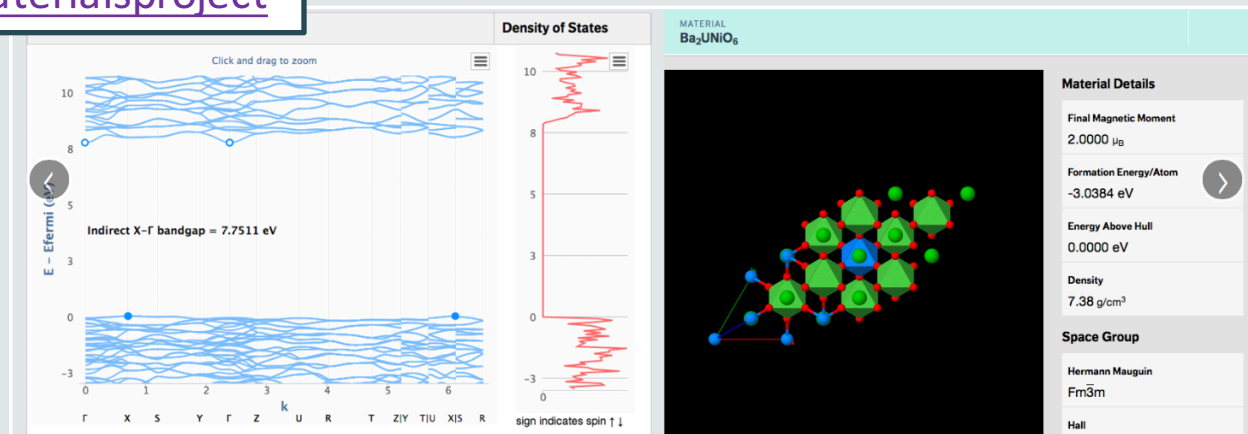
Harnessing the power of supercomputing and state-of-the-art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Learn more](#)

[Sign In or Register](#)

to start using

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



**EXPLORE  
MATERIALS**  
Search for materials

**EXPLORE BATTERIES**  
Find candidate materials  
for lithium batteries. Get

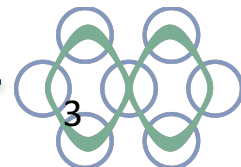
**VISUALIZE  
STABILITY**  
Generate phase and

**INVENT  
STRUCTURES**  
Design new compounds

**CALCULATE**  
Calculate the enthalpy of  
10,000+ reactions and

State-of-the-art  
OPEN SOURCE  
CODES

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

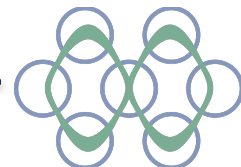


# Crystal ToolKit App & MPComplete Demo

The screenshot shows the Crystal ToolKit web application in a browser. The browser tabs include 'Materials Project', 'Material mp-1010', and 'Materials Project'. The address bar shows the URL 'https://materialsproject.org/#apps/xtaltoolkit'. The page has a dark blue header with navigation links: Home, About, Apps, Documentation, API, Tutorials, and Dashboard. Below the header is a row of icons representing various tools. The main content area is titled 'Crystal Toolkit' and features a search bar with the text 'by Material IDs' and a dropdown menu showing 'mp-604 mp-203'. Below the search bar, there is a text input field with the placeholder 'enter a space-separated list of material IDs or upload a CIF or POSCAR'. A button labeled 'Upload a POSCAR or CIF file to edit its structure' is present. A large grey box with the text 'DRAG FILES HERE' is also visible. At the bottom of the main content area, there is a logo for 'POWERED BY XSEDE' with the text 'Extreme Science and Engineering Discovery Environment'. The footer contains links for Citing, Blog, Facebook, Terms of Use, Contact, About, and API, and mentions 'Powered by pymatgen, custodian and fireworks'.

Click image or URL to  
open demo on YouTube

<https://youtu.be/k6mEA-sDSig>



# Production Workflow / FireWorks Dash

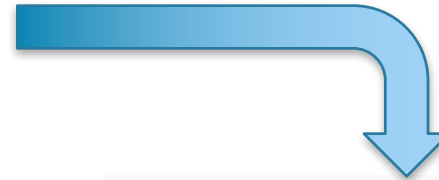
**Crystal Toolkit**

by Material IDs

enter a space-separated list of material IDs or upload a CIF or POSCAR

Upload a POSCAR or CIF file to edit its structure

DRAG FILES HERE



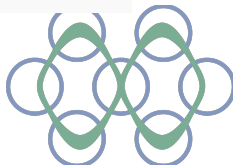
MATERIAL	ID:
<b>KNbO<sub>3</sub></b>	<b>mp-935811</b>

Submitted by **Bin Xu**

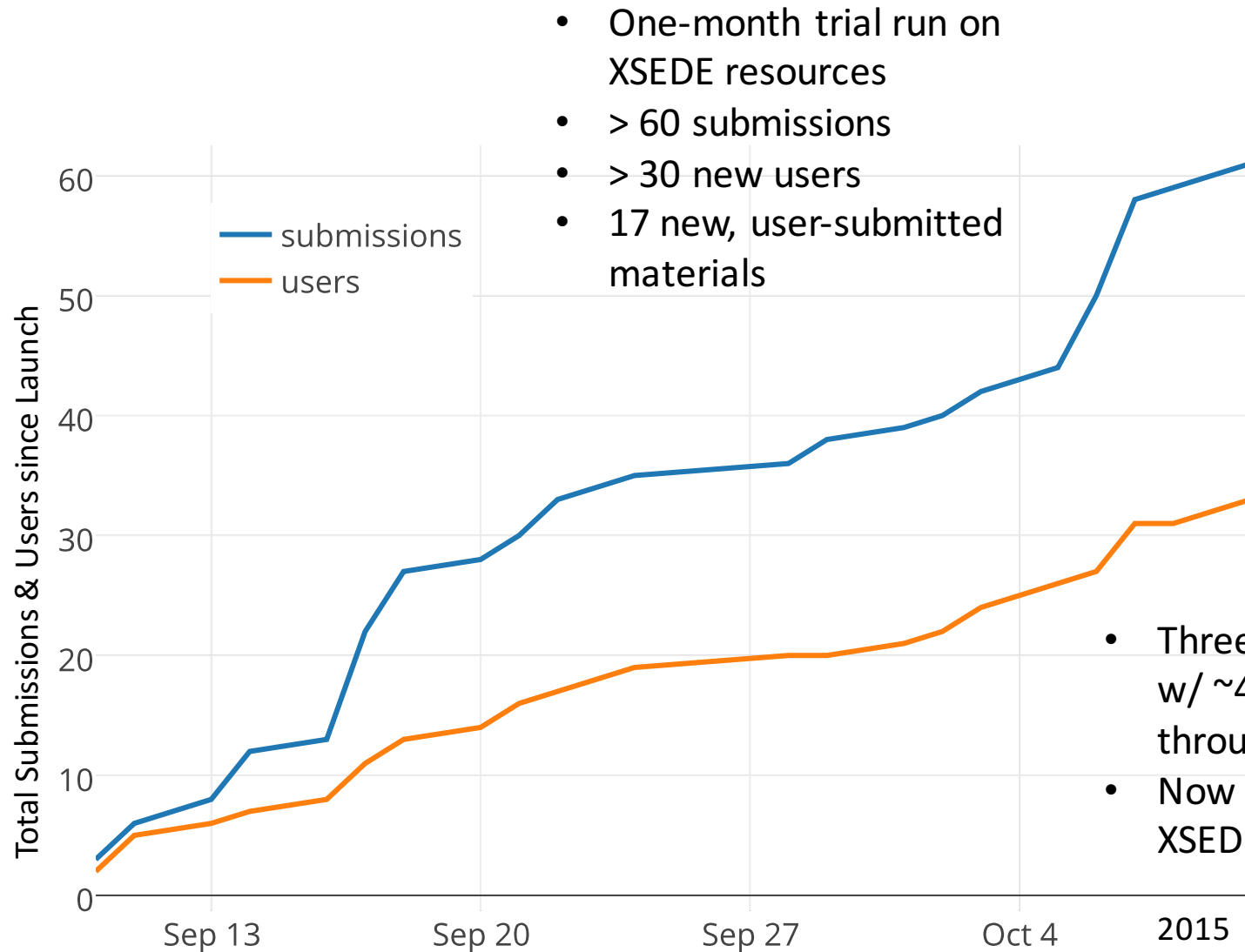
User remarks: **MP user submission**



<http://fireworks.dash.materialsproject.org/wf/1445229>

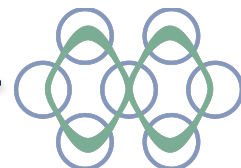


# MP-Complete Trial Run @ XSEDE



- One-month trial run on XSEDE resources
- > 60 submissions
- > 30 new users
- 17 new, user-submitted materials

- Three bulk submissions w/ ~400 structures run through NERSC
- Now transitioning back to XSEDE after extension



# Roles of MPComplete & MPContribs

Suggest new structures for calculation by MP

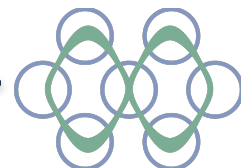
## **MPCOMPLETE**

- Assigns [new] MP identifier
- Runs calculations
- Adds material to core database

Contribute data and disseminate it through MP

## **MPCONTRIBS**

- Annotate materials already existing in core database
- Disseminate complementary theoretical and experimental data to MP users





# MP is a World-Wide Resource

**Haynes International:**  
*"The correlation between softening temperature and your calculated data is high – can we add novel alloy compositions ? "*

**Corning:** *"Thanks. Your product is astounding. I redid work that took weeks in about 15 minutes!"*

**Toyota:** *"Materials Project is a wonderful project. Please accept my appreciation to you to release it free and easy to access."*

**Cymbet:** *"I am so incredibly happy an effort like this exists now... Please please don't stop growing!"*

*"I must admit that I have always been impressed with MP and I wanted to be part of this outreach activity. I am very motivated to help anyway I can."*  
-> **Spirit of "Giving Back" across MatSci Community**

**Micron:** Your project is inspirational. Please come to Boise and educate our technical community"

553



# MPContribs: Collaborative Platform for sharing Data

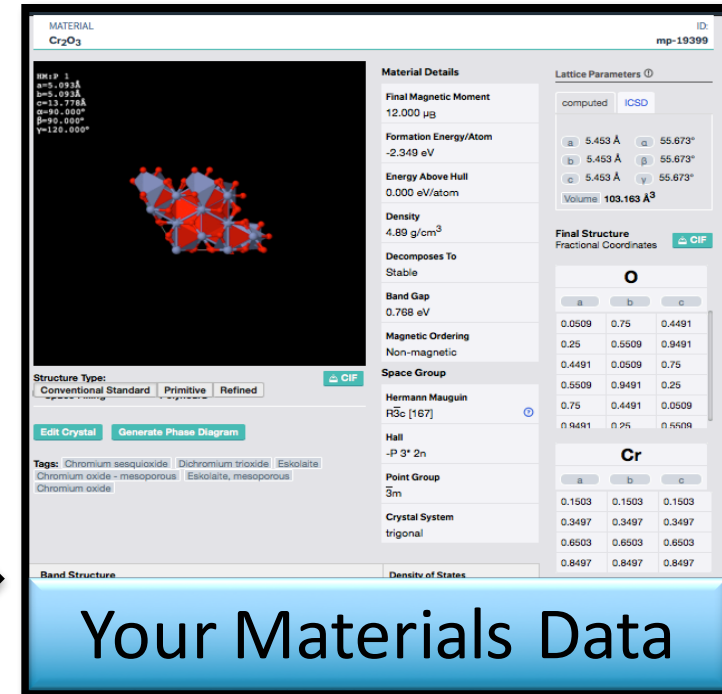
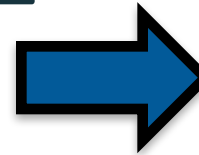
“help sharing datasets with the world”

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

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

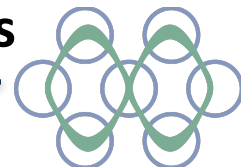
## D. Morgan, H. Wu (SI2, UW):

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

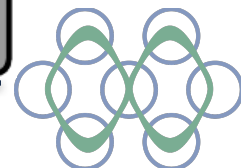
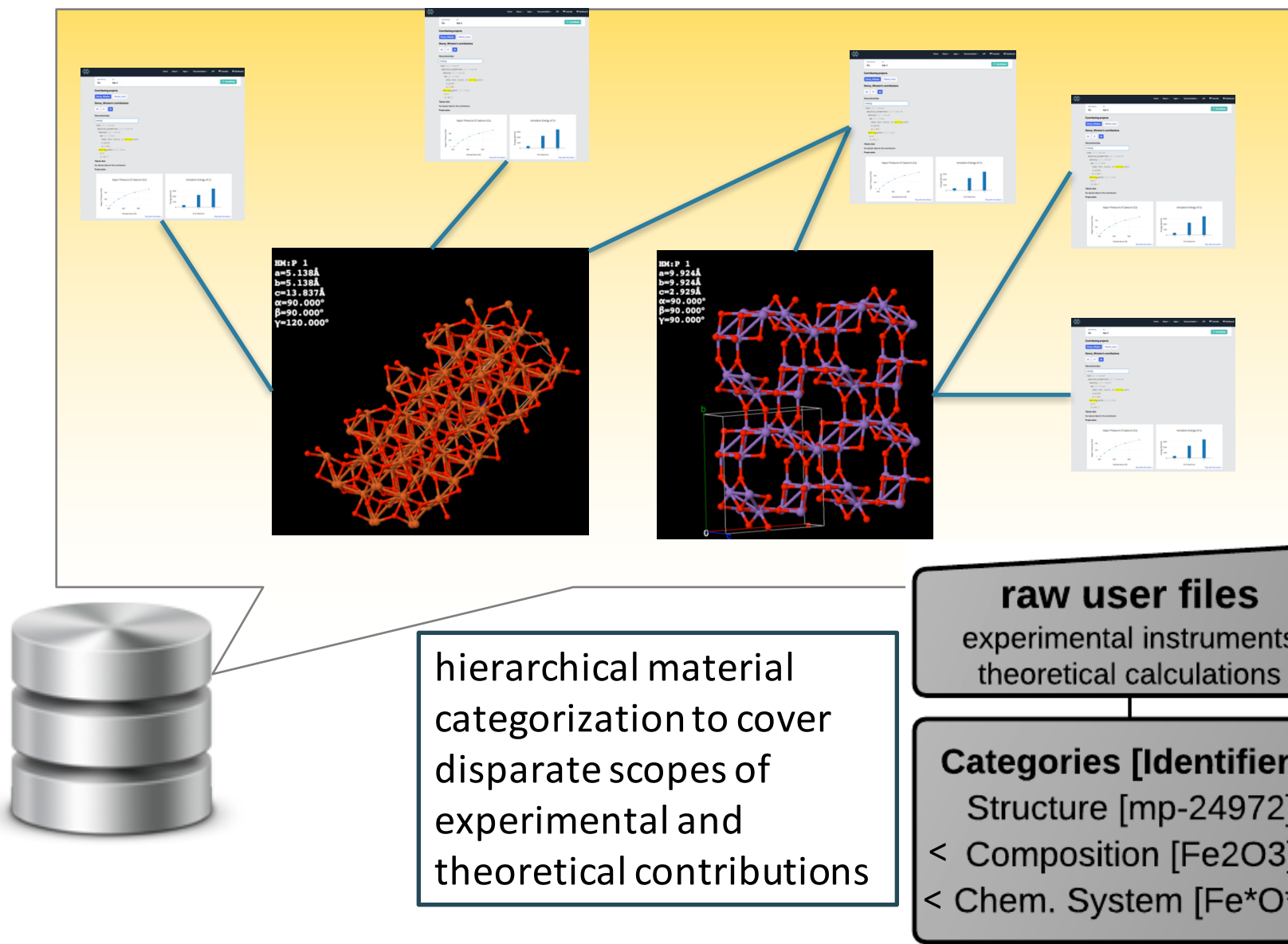


also aim to develop a customized web app driven by MPContribs

- Establish MatSci Hub for theoretical and experimental Data
- Effective dissemination for exposure to large MP user community
- > new platform to efficiently integrate data from disparate sources



# Collective Annotation of Core Database



# Correlating Contributions w/ Core Data

Hierarchical Material  
Categorization:

**raw user files**

experimental instruments  
theoretical calculations

**Categories [Identifiers]**

Structure [mp-24972]

< Composition [Fe<sub>2</sub>O<sub>3</sub>]

< Chem. System [Fe\*O\*]

Symmetry + Lattice

Specific  
compositions

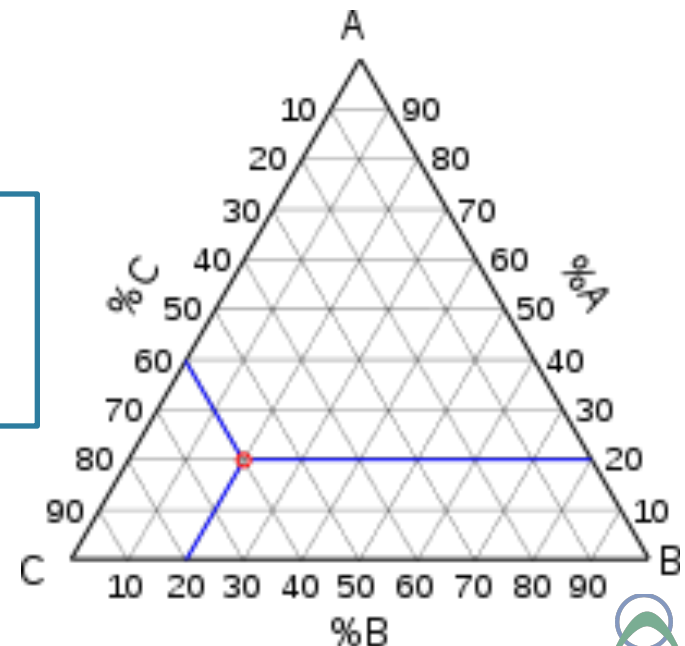
multiple  
compositions

ternary plot  
representation,  
e.g. phase  
diagrams

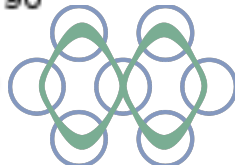
materials/mp-24972/contributions  
(mostly theoretical contributions)

links to

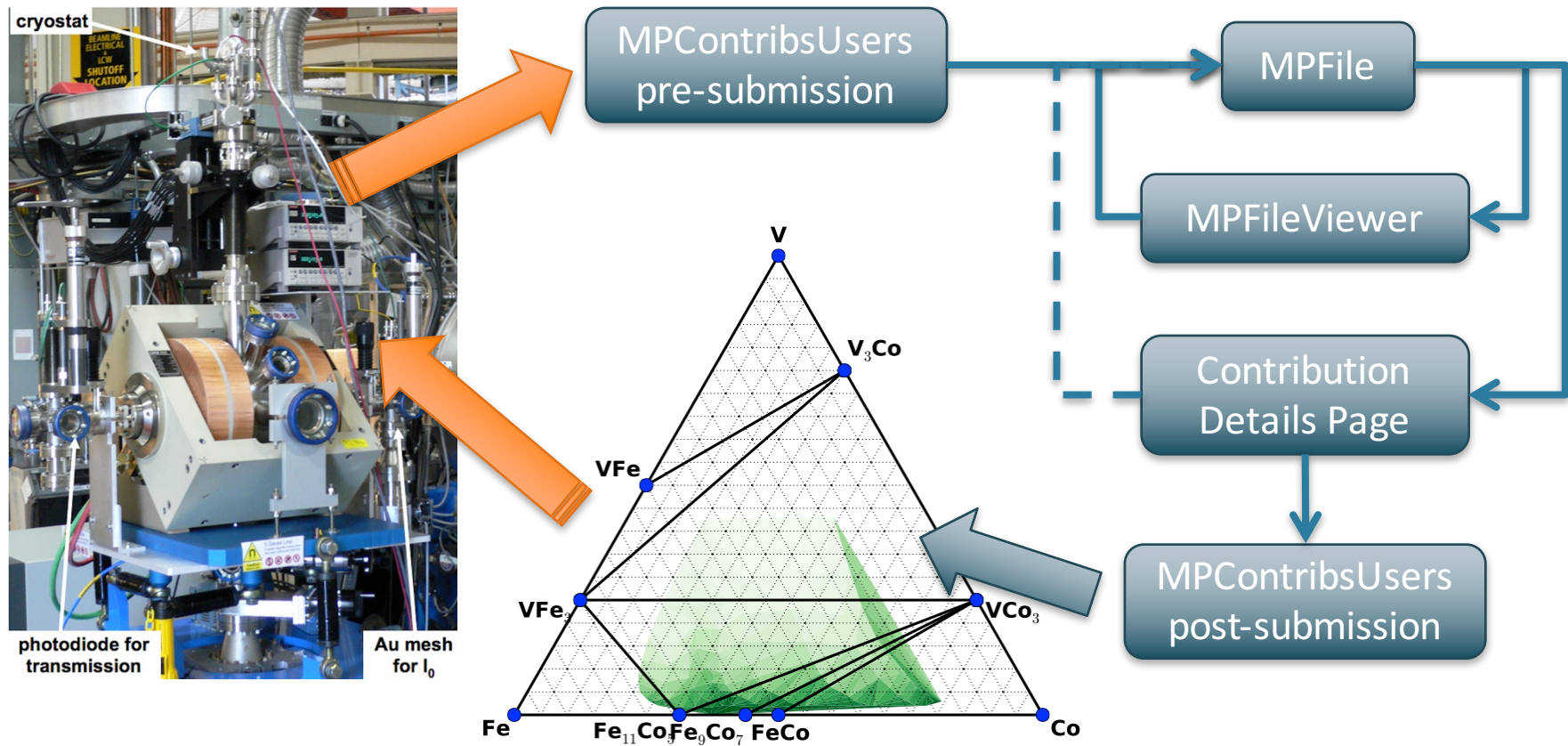
compositions/Fe<sub>2</sub>O<sub>3</sub>/contributions  
(experimental contributions)



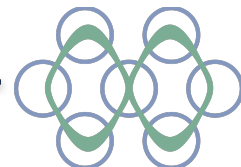
SHOWCASE: **Unified Experimental and Theoretical XAS  
Application** [see paper at 10<sup>th</sup> GCE workshop]



# MPContribs User Workflow



- pre-processing of user output data and conversion into MPFile
- visual and iterative checking of MPFile by user ("get data in shape")
- MPFile submission via command line or web portal (through REST)
- contributed data appears instantly on the MP portal



# Offline Web UI – “Get Data in Shape”

[Home](#)[ArchieML ▾](#)[Choose MPFile ...](#)[Load MPFile](#)[View MPFile](#)[View Graphs](#)[Save MPFile](#)[Contribute](#)[Quit](#)

locally process contribution #0 ... OK.  
check consistency of contribution #0 ... OK.  
build contribution #a898b40 into Fe8Ni2Pt ... OK.  
**1 contributions successfully processed.**

[Go to contribution ... ▾](#)

## Fe8Ni2Pt » Patrick Huck » #a898b40

### Hierarchical Data

▼ (root): {} 3 Items

▼ Experiment: {} 4 Items

► Preparation: {} 1 Item

▼ Sample: {} 5 Items

Material\_Name: Platinum doped Permalloy

Form: ~20nm film on Si wafer

Thickness: ca. 20nm with 2-3 nm Au-capping (nominally)

Grower: Ales Hrabec

Authors: Ales Hrabec, Alpha T. N'Diaye, Elke Arenholz, Christopher Marrows

► Measurement: {} 5 Items

► Beamline: {} 7 Items

▼ Ni\_XMCD: {} 2 Items

► get\_xmcd: {} 1 Item

▼ xas\_normalization\_to\_min\_and\_max: {} 3 Items

energy\_range: 800 1000

normalization\_factor: 0.952002315041

offset: 0.358620768783

► Fe\_XMCD: {} 3 Items

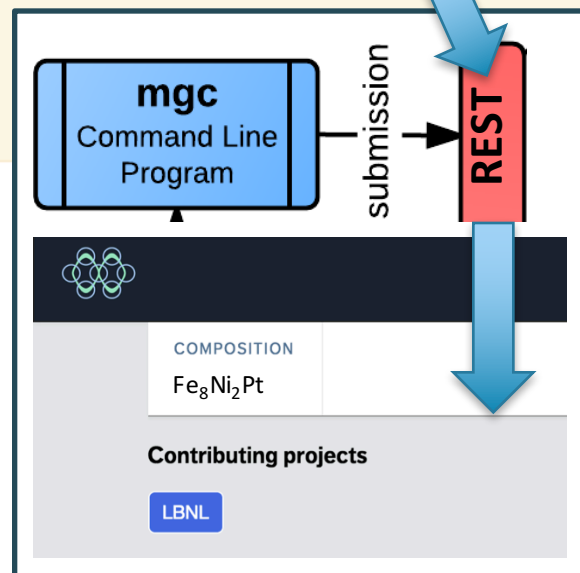
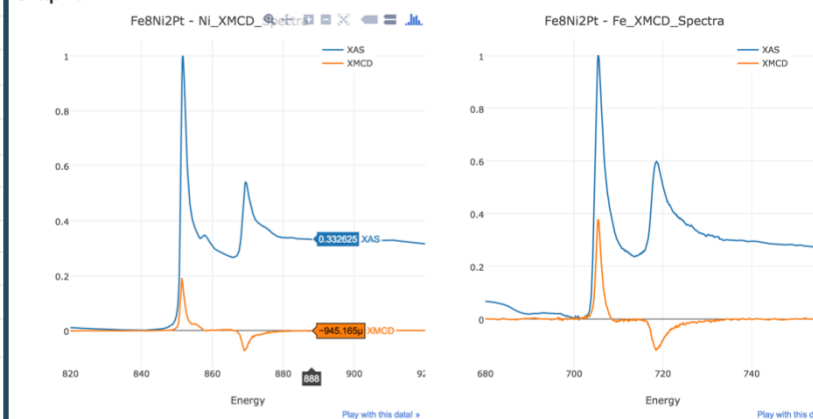
### Tables

data\_Ni\_XMCD\_Spectra [Collapse/Expand](#)

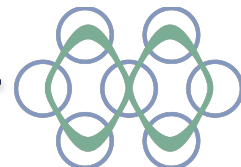
Search:

Energy ↓↑	XAS ↑↑	XMCD ↓↑
821.0	0.0104183	-0.000451802
822.0	0.00931404	-0.000974055

### Graphs



Demo: <https://youtu.be/xlwttmXSpHg> (Full Playlist)





# Offline Web UI – Release-Ready Demo

The screenshot displays the MPContribs Framework web interface. At the top, there's a navigation bar with the logo and several buttons: 'MPFile ...', 'Load MPFile', 'View MPFile', 'Save MPFile', and 'Contribute'. Below the navigation bar, the main content area is divided into several sections.

**Code Editor:** A Jupyter/IPython cell on the left contains the following code:

```
1 %load_ext autoreload
2 %autoreload 2
3 from mpcontribs.io.archieml.mpf import MPFile
4 mpfile = MPFile.from_file()
5 # Load pre-submission processing of "atn" project
6 from mpcontribs.users.atn.pre_submission import run
7 run(mpfile)
8 mpfile.write_file()
```

**Progress Bar:** Below the code editor, a progress bar shows 100% completion, with a value of 120/120 and a time of 00:09:00:00, 12.66it/s.

**Data Table:** A table displays the results of the processing:

No.	Co (at%)	V (at%)	Fe (at%)	Total	Xnom (mm)	Ynom (mm)	
0	1	76.8	1.7	21.5	100	1	23
1	2	75.5	2.1	22.4	100	1	21
2	3	74.1	2.6	23.3	100	1	19
3	4	72.8	3.1	24.1	100	1	17
4	5	71.0	4.1	24.9	100	1	15

**Buttons:** A 'Run Again' button is located below the table. A 'Save Code' button is also present.

**Instructions:** A yellow box on the right provides instructions:

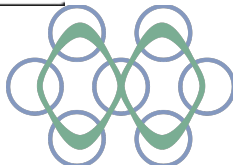
- Editable and runnable Jupyter/IPython cell on the left.
- Use **Run / Run Again** or **shift + return** to execute.
- MPFile I/O is handled automatically by **from/write\_file()**.
- Resulting output MPFile is used for **View MPFile**.
- Click **Load MPFile** to reload MPFile from ArchieML Sandbox.
- Click **Save Code** below to preserve your code changes.
- Start from scratch by clicking the logo.

**JSON Output:** A live-preview of the JSON representation after default ArchieML parsing is shown at the bottom right:

```
{
  "Experiment": {
    "Preparation": "Sputter deposition",
    "Sample": {
      "Material": "Vicalloy",
      "Form": "~100nm film on Si wafer",
      "Thickness": "ca. 20nm with 5 nm Pt-capping (nominally)",
      "Authors": "Please Contact Alpha T. N'Diaye (atndiaye@lbl.gov)"
    }
  }
}
```

**Annotations:** A blue box on the right contains the text: 'Click image or URL to open demo on YouTube'. Below it, a blue box contains the URL: <https://youtu.be/zH-ZauYsu64>.

**Text Overlay:** The text 'modify and rerun pre-submission processing' is overlaid on the bottom left of the image.



# ALS MPFile: Labbook & Processing Control

Experiment.Preparation.Description: Sputter deposition

{Experiment.Sample}

Material\_Name: Platinum doped Permalloy

Form: ~20nm film on Si wafer

Thickness: ca. 20nm with 2-3 nm Au-capping (nominally)

Grower: Ales Hrabec

Authors: A. Hrabec, A. T. N'Diaye, E. Arenholz, C. Marrows

{Experiment.Measurement}

Detection: total electron yield

Temperature: RT

Orientation: 30° grazing incidence

Date: 2015-06-24

Measured\_by: Alpha T. N'Diaye

**Shared Meta-Data  
(from Labbook)**

{Experiment.Beamline}

Beamline: ALS-6.3.1

Method: Soft x-ray XAS and XMCD

Polarization: circular, positive (ca. 60%)

Magnet\_Field: 0.8T switching point by point, parallel to beam

Count\_Time: 1s

Delay\_Time: 0.5s

Monochromator.Exit\_Slit: 20µm

Monochromator.Grating: 600l/mm

**MPFile = Config + Input + Output**

- Default interactive graphs from each data table
- Check results & reiterate via **Offline Web UI**
- *Future*: guide user in what to include as Meta-Data

{Ni20Fe80Pt10}

Ni\_XMCD.get\_xmcd.energy\_range: 800 1000

Fe\_XMCD.get\_xmcd.energy\_range: 600 800

{Ni20Fe80Pt10.Ni\_XMCD.xas\_normalization\_to\_min\_and\_max}

energy\_range: 800 1000

normalization\_factor: 0.952002315041

offset: 0.358620768783

**Raw Data  
Processing  
Instructions**

{Ni20Fe80Pt10.Fe\_XMCD.scaling\_preedge\_to\_1}

preedge\_range: 690 700

xas\_minus\_factor: 0.348231766387

xas\_plus\_factor: 0.349333591384

**Results of  
Processing  
Steps**

{Ni20Fe80Pt10.Fe\_XMCD.xas\_normalization\_to\_min\_and\_max}

energy\_range: 600 800

normalization\_factor: 1.00964185927

offset: 0.984095999176

[+Ni20Fe80Pt10.Ni\_XMCD\_Spectra]

Energy, XAS, XMCD

820, 0.0104944, -0.00140602

821, 0.0104183, -0.000451802

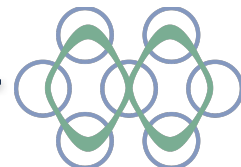
822, 0.00931404, -0.000974055

823, 0.00821621, -0.00083305

**Final XAS  
Spectra (CSV)**

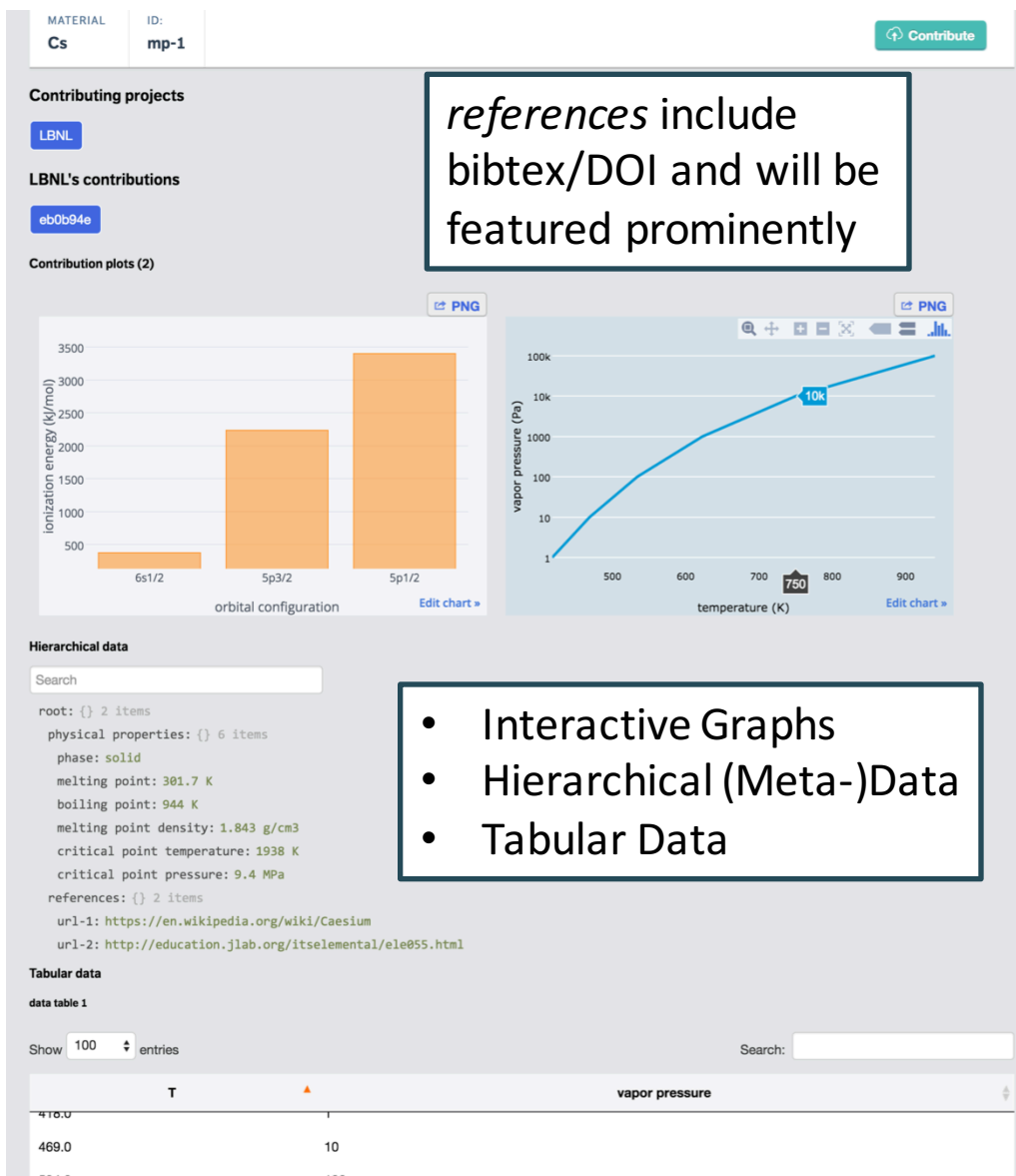
[+Ni20Fe80Pt10.Fe\_XMCD\_Spectra]

Energy, XAS, XMCD





# MPFile & Generic Contribution Details Page



```
{mp-1.physical_properties} for caesium
phase: solid
melting_point: 301.7 K
boiling_point: 944 K
melting_point_density: 1.843 g/cm3
critical_point_temperature: 1938 K
critical_point_pressure: 9.4 MPa
```

```
[mp-1.references] list of url, bibtex, or doi
* https://en.wikipedia.org/wiki/Caesium
* http://education.jlab.org/itselemental/ele055.html
```

```
{mp-1.plots.default_data_table2} overwrite graph props
x: configuration
y: ionization energy
kind: bar
table: table2
```

```
[+mp-1.table1] can be named freely
T, vapor pressure
418,1
469,10
534,100
623,1000
750,10000
940,100000
```

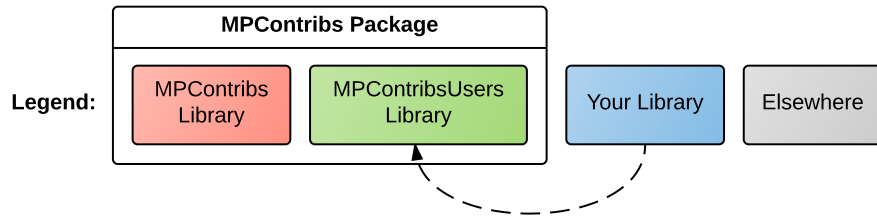
ArchieML as  
MPFile format

```
[+mp-1.table2]
electron number, ionization energy, configuration
1,375.7,6s1/2
2,2234.3,5p3/2
3,3400,5p1/2
```

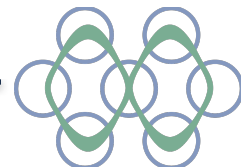
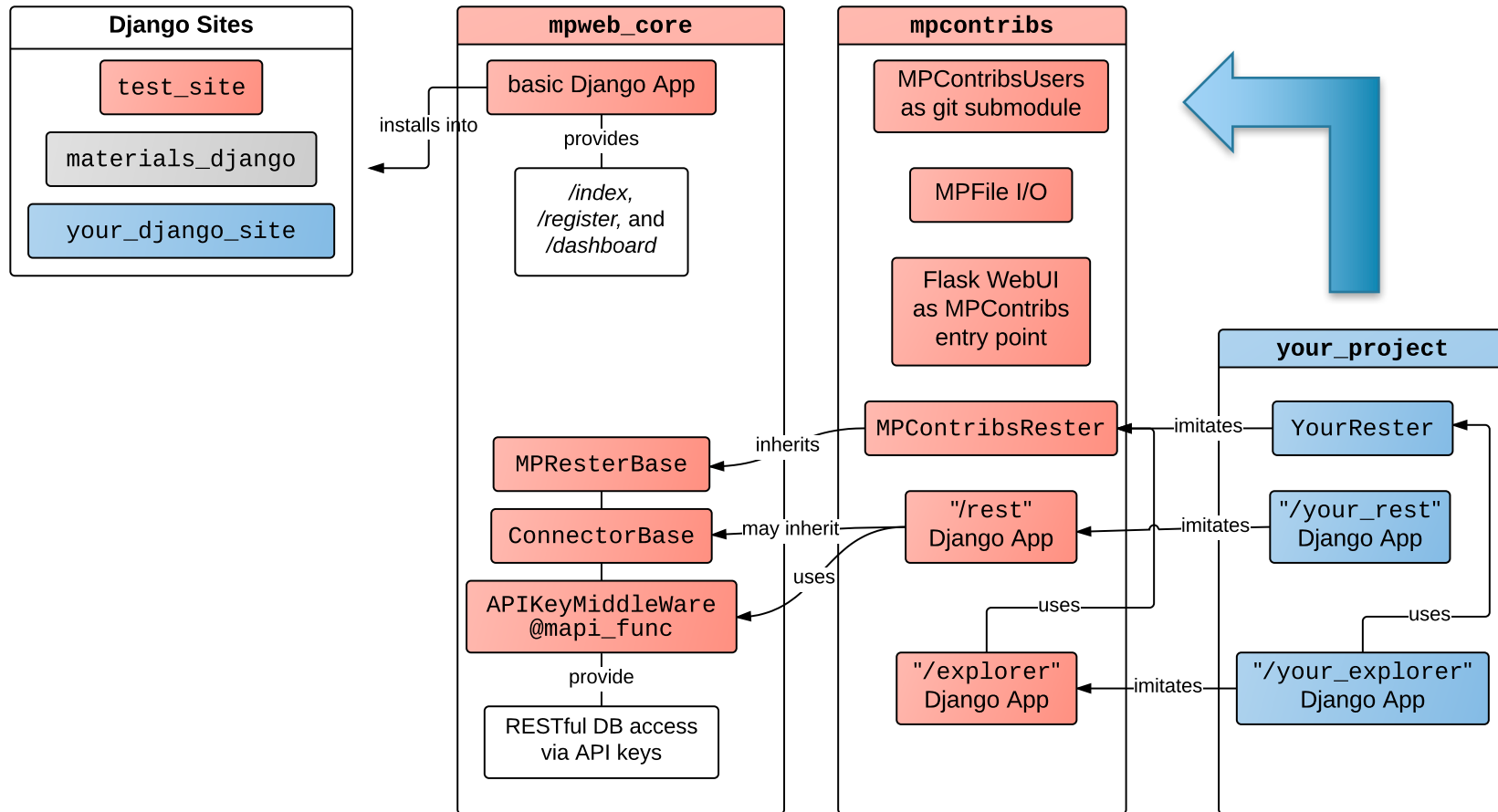
```
[+mp-2] bare data section for palladium
temperature (K), vapor pressure (Pa)
```



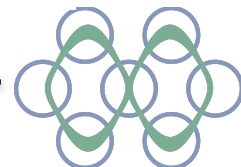
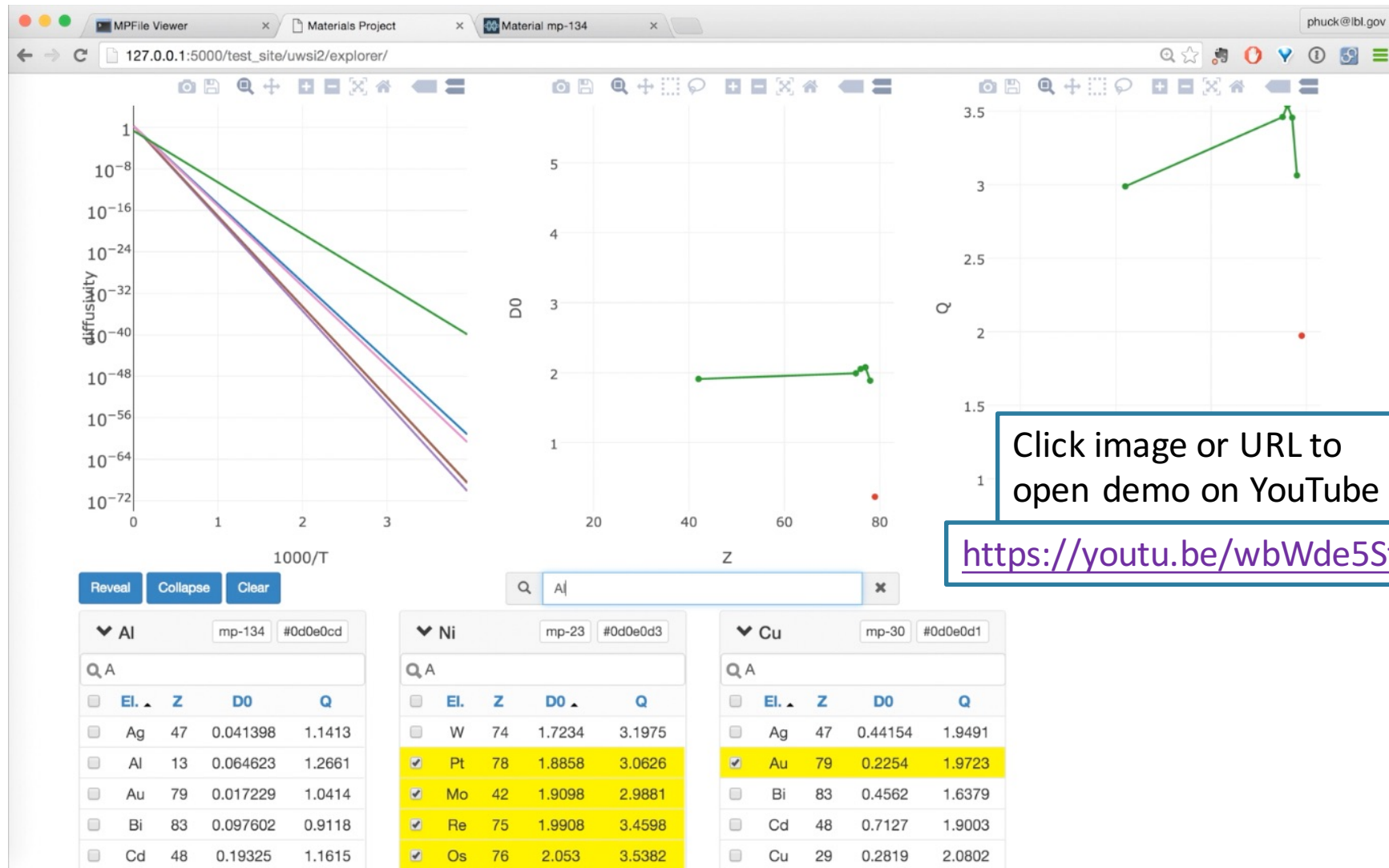
# MPContribs Software Components



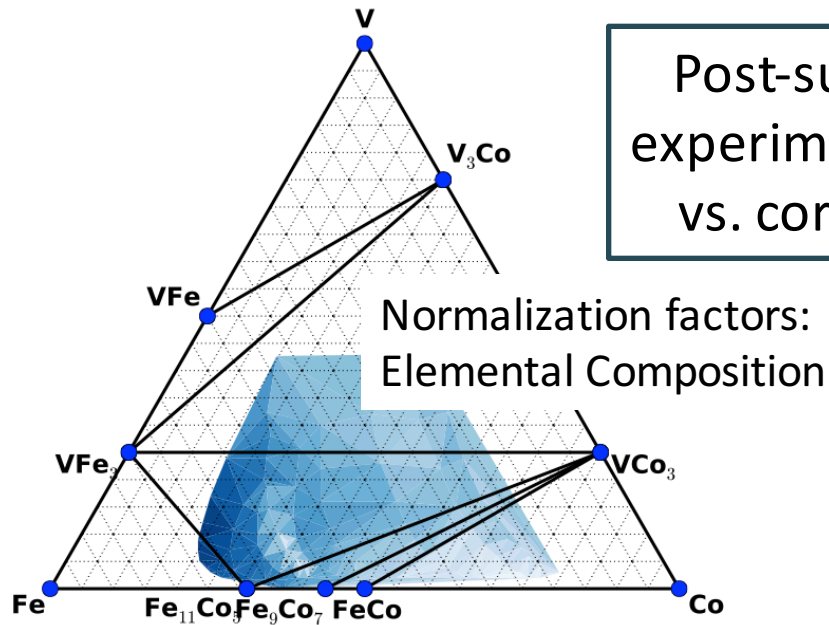
Reusable user  
web apps  
powered by MP



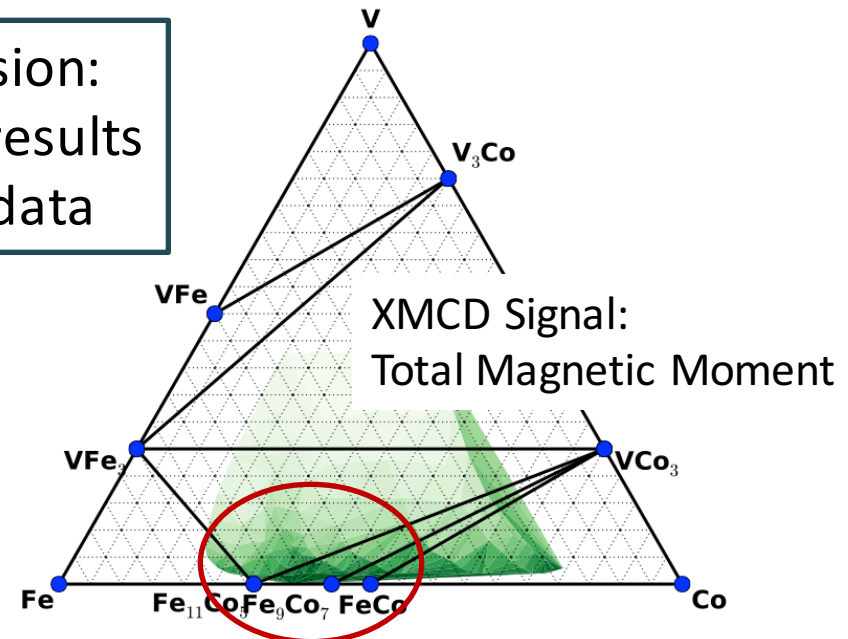
# UW/SI2 Diffusion App - Demo



# XMCD/Magnetic Moment – Phase Diagram



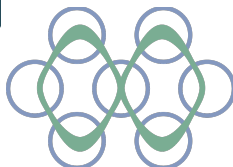
Post-submission:  
experimental results  
vs. core MP data



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

**MPCONTRIBS** helps contributor to

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



# Conclusions

*User-contributed data will play an important role in expanding MP towards serving a larger community (wait-list!).*

## **MPComplete:**

- Underpins MP's Crystal ToolKit App
- Enables user suggestions of new structures for calculation by MP
- MP production at NERSC, but user submissions at XSEDE

## **MPContribs:**

- Software platform for users to share data with >14k users
- Extend core data with user-curated and -contributed data
- Data preparation, interactive graphing & integrated analyses
- Combine contributions and instantly serve on generic frontend
- Basis for other projects to build custom web applications

Docs: <http://pythonhosted.org/mpcontribs/>  
GitHub: <https://github.com/materialsproject/MPContribs>

# Thanks!

Demo: <https://youtu.be/xlwttmXSpHg> ([Full Playlist](#))

