Effective and interactive dissemination of diffusion data using MPContribs

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MGI & Materials Project: Achievements to Date

Materials Genome Initiative

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

"solutions in most pressing areas require advanced materials"

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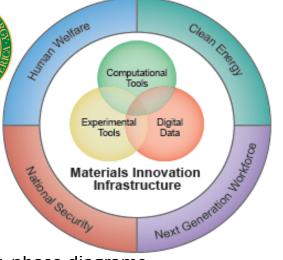
High-Quality Materials DATA

Rapid DISSEMINATION

DESIGN

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



MP Web Site – A Science Gateway



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

Sign In or Register to start using Learn more

Density of States Ba₂UNiO₆ Click and drag to zoon Material Details Final Magnetic Moment 2.0000 µB Formation Energy/At -3.0384 eV Energy Above Hull Indirect X-F bandgap = 7.7511 eV Efer 0.0000 eV <u>ل</u> Density 7.38 a/cm3 Space Group Fm3m sign indicates spin 1 Hal

EXPLORE **EXPLORE BATTERIES** VISUALIZE INVENT CALCULATE MATERIALS Find candidate materials **STABILITY STRUCTURES** Search for materials for lithium batteries. Get Generate phase and Design new compounds voltage profiles and information by chemistry, pourbaix diagrams to find with our structure editor compare with composition, or property oxygen evolution data. stable phases and study and substitution experimental values reaction pathways algorithms

State-of-the-art **OPEN SOURCE** CODES

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

Calculate the enthalpy of 10,000+ reactions and

Contribute data and disseminate it through MP

MPCONTRIBS

"help sharing datasets with the world"

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

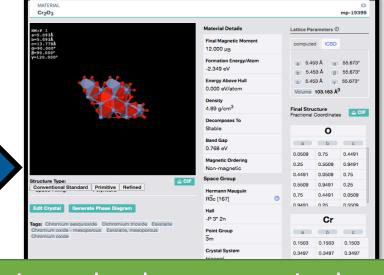
- measured XAS/XMCD spectra
- properties of rare earth substitutes
- processing of instrumental data
- integration w/ MP phase diagrams

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



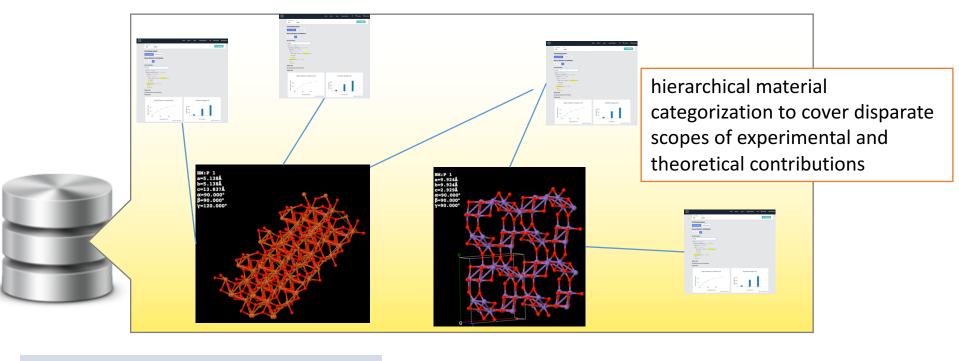
aim to develop a customized web app driven by MPCONTRIBS

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

Huck P. et al.; eScience15; GCE15; Poster; MRS16 Spring & Fall

full contributors list

Collective Annotation of Core Database



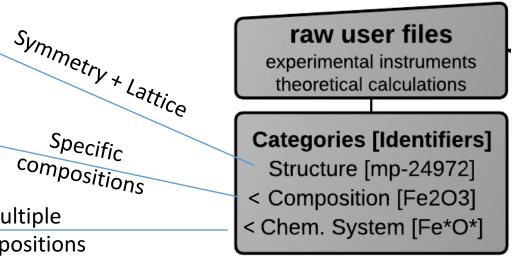
materials/mp-24972/contributions (mostly theoretical contributions)

links to compositions/Fe2O3/contributions (experimental contributions)

> ternary plot representation, e.g. phase diagrams

compositions multiple compositions

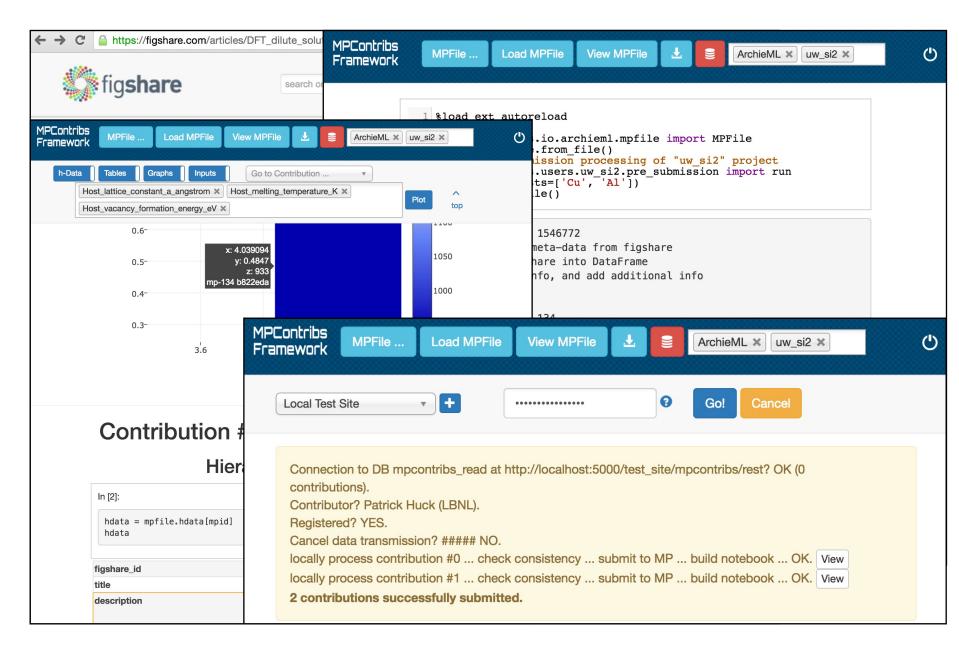
Specific



Integration with JupyterHub

Jupyter Hub	× C MPContribs	× phuck@lbl.gov				
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	/mpcontribs/rest	REST API docs & test queries for public DB				
Materials Project Alpha Site at <u>http://alpha.materialsproject.org</u>	/mpcontribs/explorer	Explore data contributed to public DB				
	/uwsi2/explorer	Custom interface to contributed public UW/SI2 data				
	L	Landing page with OrgTable (this page)				
	<u>/ingester</u>	Data ingestion, preparation, and DB submission				
	<u>/test_site</u>	Local MP-like Django test site				
All MPContribs services available to user in private Local/MP JupyterHub Instance at /flaskproxy/tschaume/	/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/uwsi2/explorer	Custom Interface to contributed private UW/SI2 data				

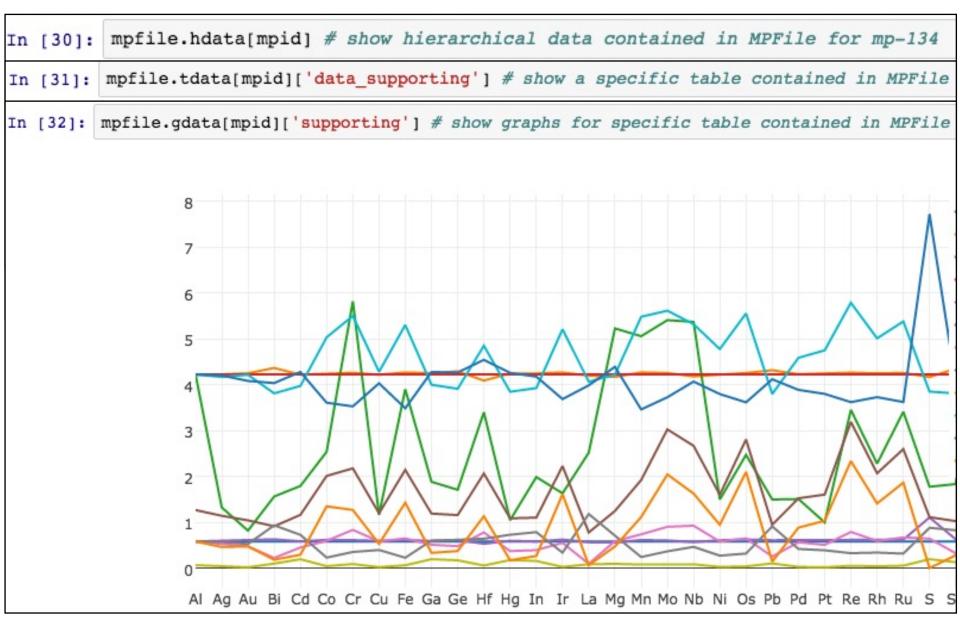
Data Preparation, Ingestion & Submission



Explorer & REST Interfaces

		Home Dashboard Logo	ut									
Explo	ore contribute	ed Materials or Compositions ?										
Selec	t (one or mo	ore) materials and/or projects:										
Sele	ct material(s)	LBNL × Find										
Or en	ter a (list of)	contribution identifiers:										
Ente		ID(a) Chaw										
	In [26]:	from mpcontribs.rest.rester import MPContribsRester										
Resul /test_ /test_		<pre>SITE = 'http://localhost:5000/test_site' # or http://alpha.materialsprojed API_KEY = 'Gn6tOpaHM1EAsbTr' # copy from SITE dashboard ENDPOINT = SITE + '/mpcontribs/rest' # REST API endpoint for SITE mpr = MPContribsRester(API_KEY, endpoint=ENDPOINT)</pre>	t.org									
	<pre>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)</pre>											
	In [29]:	<pre>mpfile = mpr.find_contribution(cid) # get MPFile object from MPContribsRes mpid = mpfile.ids[0] # MP material identifier (e.g. mp-134)</pre>	ter									

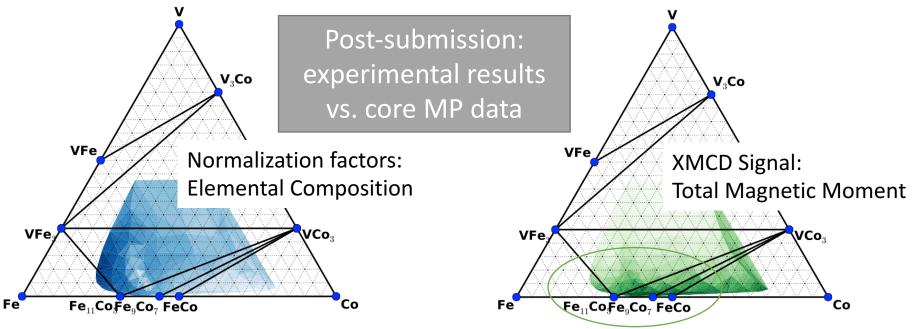
MPFile Components



UW/SI2 Diffusion App - Demo

MPFile V	liewer	×	Materials F	Project	×	Mat	terial mp-134	×						phuck@lbl.gov
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🔲 AI	13	0.064623	1.2661	6	Pt	78	1.8858	3.0626	Ø	Au	79	0.2254	1.9723	
	79	0.017229	1.0414	6	🛛 Mo	42	1.9098	2.9881		Bi	83	0.4562	1.6379	
🗆 Au														
Au Bi	83	0.097602	0.9118	6	Re	75	1.9908	3.4598		Cd	48	0.7127	1.9003	

XMCD/Magnetic Moment 👄 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

