

# Interactive Leaderboard for Requesting and Tracking Expensive Calculations of Optional Properties across a Database of Materials

Donny Winston, Joseph Montoya, and Kristin Persson

Lawrence Berkeley National Laboratory

Science Gateways Conference, SDSC, San Diego, CA

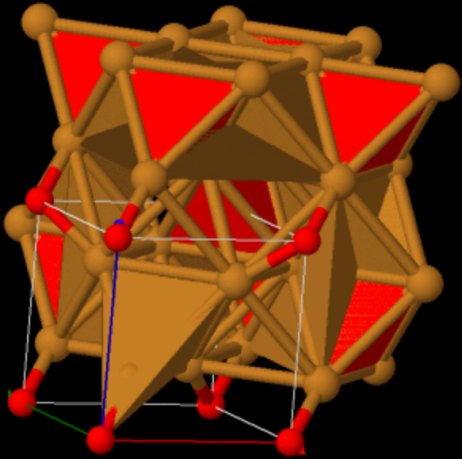
November 2, 2016

# A database of inorganic crystalline material structures and properties

MATERIAL ID: DOI:

**Cu<sub>2</sub>O** **mp-361** **10.17188/1207131**

HM: P 1  
 a=4.288Å  
 b=4.288Å  
 c=4.288Å  
 α=90.000°  
 β=90.000°  
 γ=90.000°



**Material Details**

**Final Magnetic Moment**  
0.000 μ<sub>B</sub>

**Magnetic Ordering**  
Unknown

**Formation Energy / Atom**  
-0.650 eV

**Energy Above Hull / Atom**  
0.000 eV

**Density**  
6.03 g/cm<sup>3</sup>

**Decomposes To**  
Stable

**Band Gap**  
0.500 eV

Reference for tensor and properties: [📖](#) [Visualize with ELATE](#)

**Stiffness Tensor C<sub>ij</sub> (GPa)**

124.16	105.26	105.27	0	0	0
105.26	124.17	105.27	0	0	0
105.27	105.27	124.18	0	0	0
0	0	0	7.69	0	0
0	0	0	0	7.69	0
0	0	0	0	0	7.69

**Compliance Tensor S<sub>ij</sub>**

<b>Shear Modulus G<sub>V</sub></b>	<b>Bulk Modulus K<sub>V</sub></b>
8.40 GPa	111.57 GPa
<b>Shear Modulus G<sub>R</sub></b>	<b>Bulk Modulus K<sub>R</sub></b>
8.31 GPa	111.57 GPa
<b>Shear Modulus G<sub>VRH</sub></b>	<b>Bulk Modulus K<sub>VRH</sub></b>
8.35 GPa	111.57 GPa
<b>Elastic Anisotropy</b>	<b>Poisson's Ratio</b>
0.05	0.46

Structure Type: [Conventional Standard](#) [Primitive](#) [Refined](#) [CIF](#)

<https://www.materialsproject.org>

Some calculated properties are useful but computationally expensive

### Database Statistics

**67,403**

INORGANIC COMPOUNDS

**52,284**

BANDSTRUCTURES

**21,954**

MOLECULES

**530,243**

NANOPOROUS MATERIALS

**3,408**

ELASTIC TENSORS

**941**

PIEZOELECTRIC TENSORS

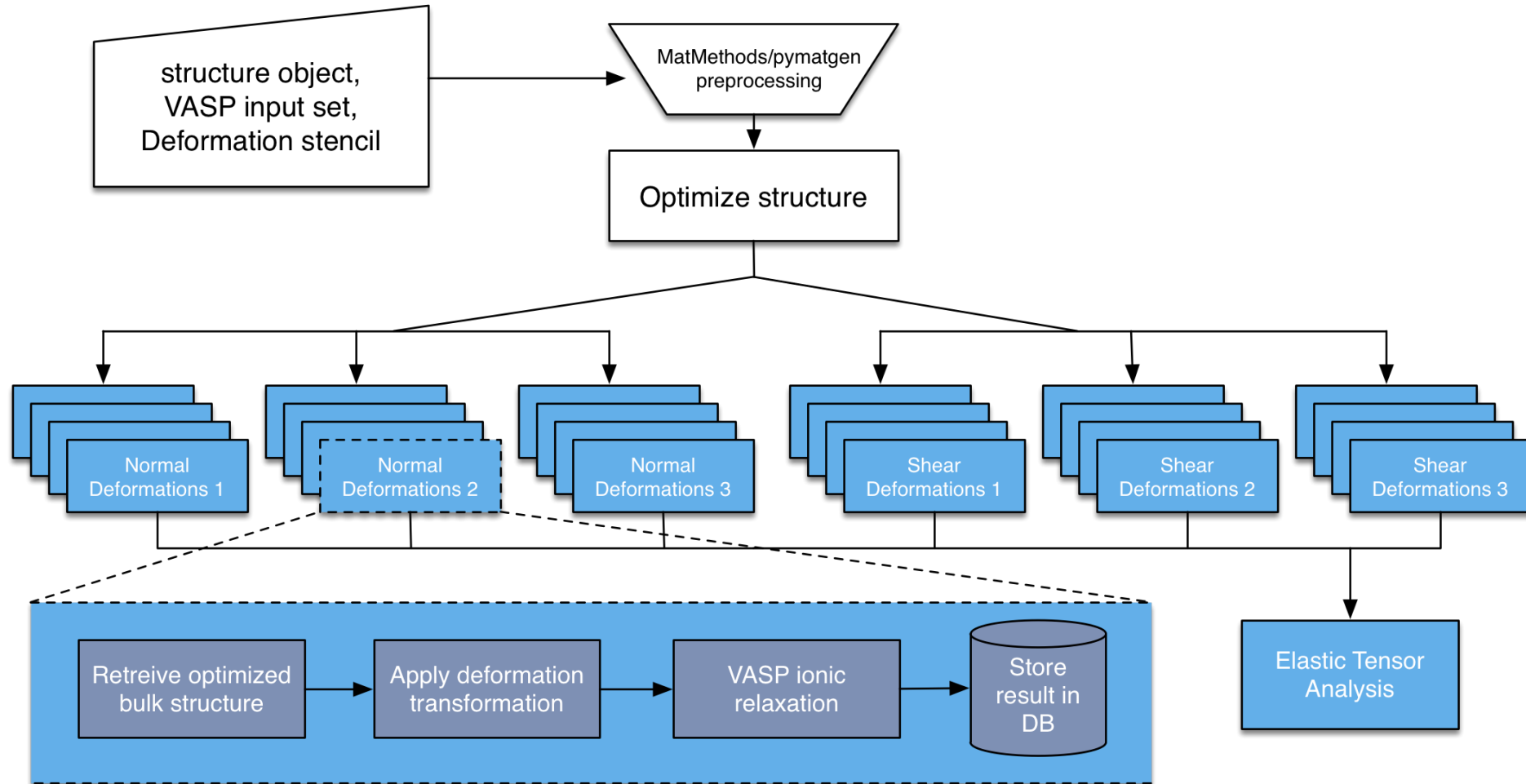
**3,628**

INTERCALATION ELECTRODES

**16,128**

CONVERSION ELECTRODES

# A workflow for calculating a full elastic tensor



# Entice users with a hook

## Elasticity

A full elastic tensor has not been calculated for this material. Would you like [statistical-learning-based](#) predictions of this material's bulk and shear moduli?

By clicking the button at right, you are also "voting" for full calculation of this material's elastic properties.

Reference for predictions:



Get predictions

**Bulk Modulus**  
 **$K_{VRH}$**

139.88 GPa

**Shear Modulus**  
 **$G_{VRH}$**

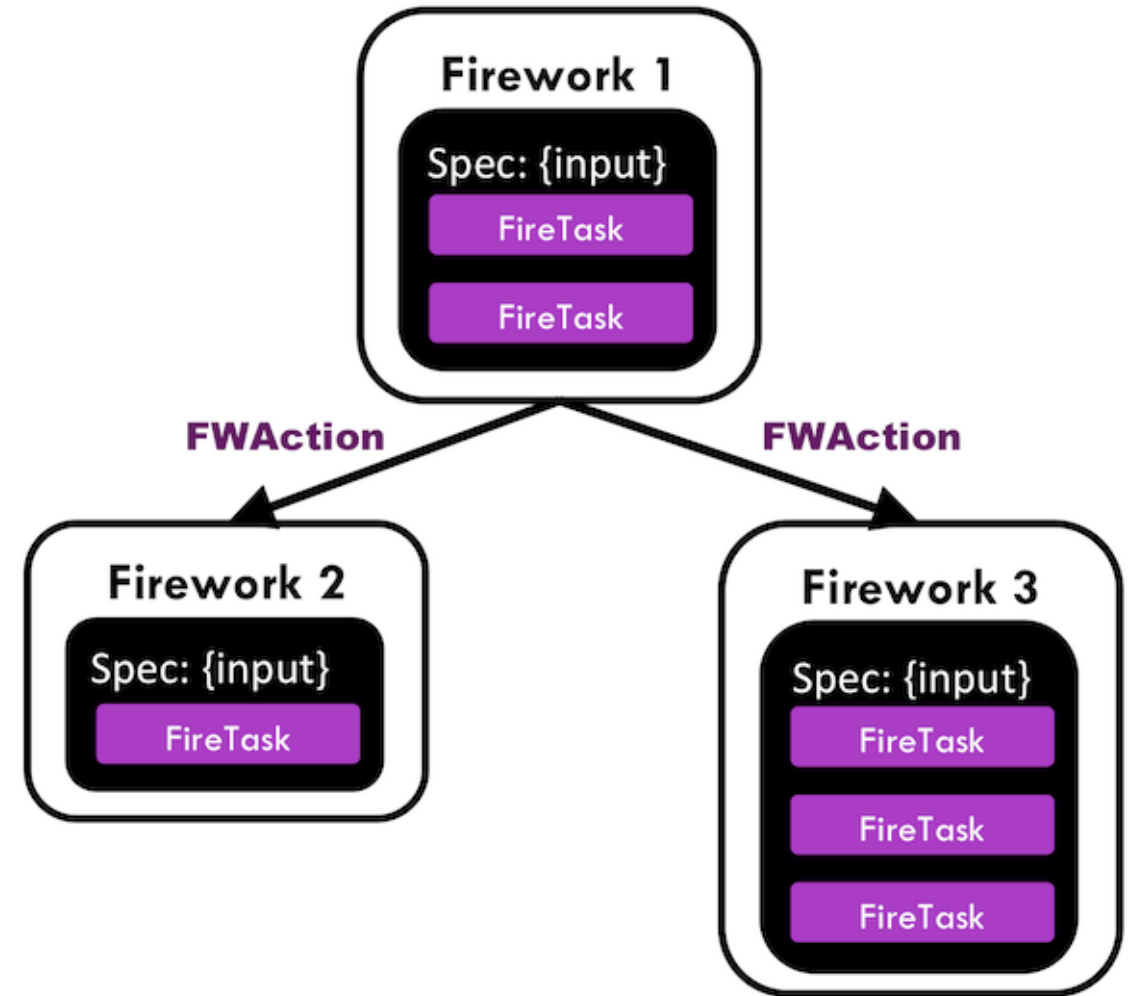
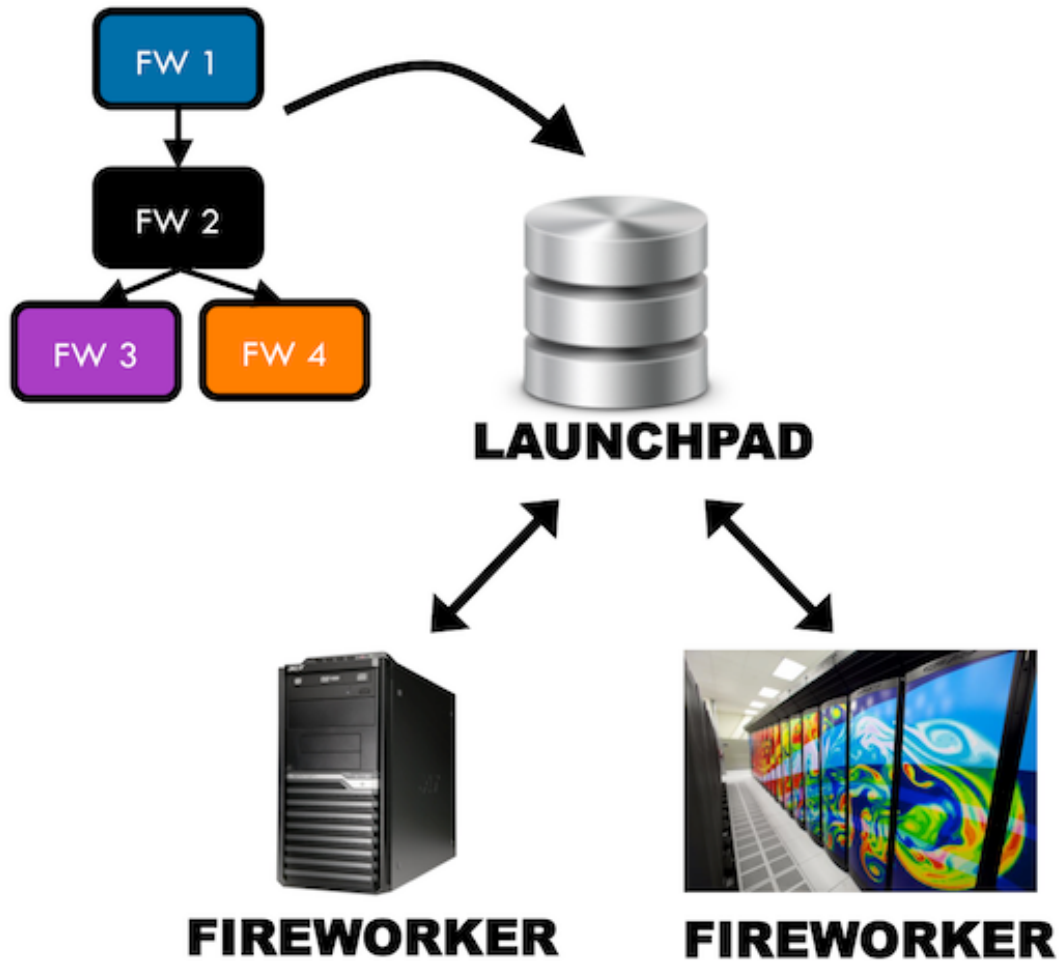
76.12 GPa

ⓘ **Warning:** [?] Predictions may be less reliable for materials with non-GGA runs.


doi:10.1038/srep34256

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

FireWorks helps define workflows with database-backed state, provenance, and priority



# FireWorks has built-in web-based monitoring



## Workflow Dashboard

**Newest Workflows**

Cr1 Si1 Te3 READY ID: 173672

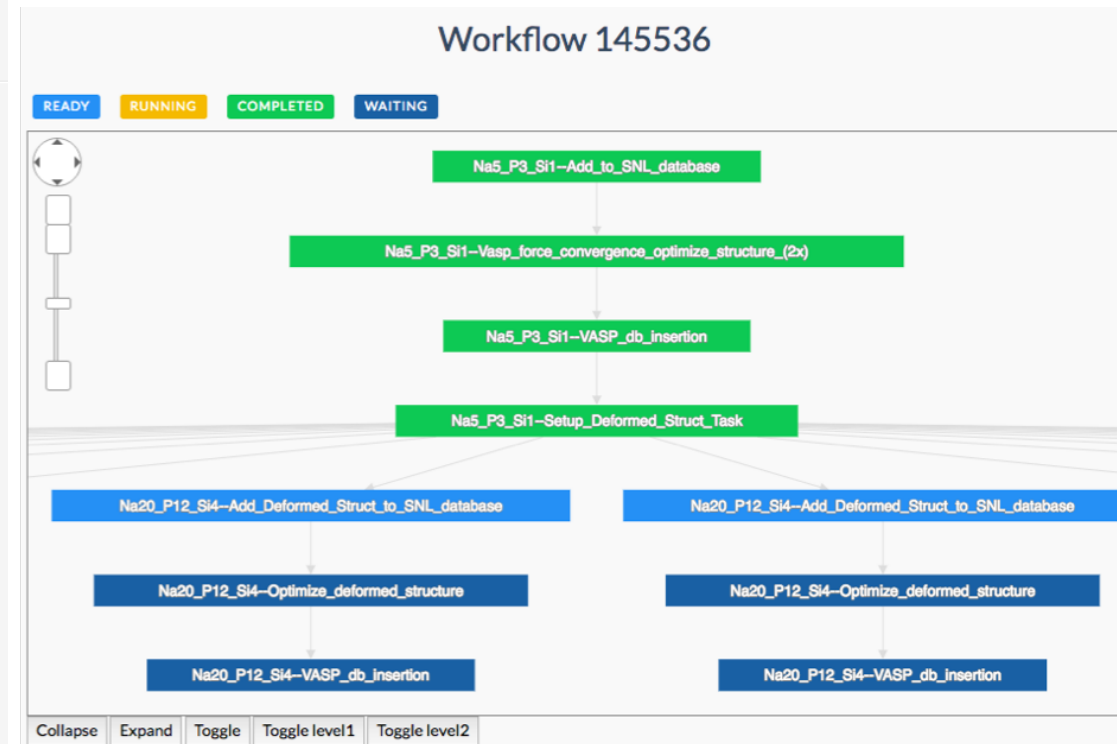
- Cr1\_Si1\_Te3--Setup\_Deformed\_Struct\_Task
- Cr1\_Si1\_Te3--VASP\_db\_Insertion
- Cr1\_Si1\_Te3--Vasp\_force\_convergence\_optimize\_structure\_(2x)
- Cr1\_Si1\_Te3--Add\_to\_SNL\_database

Al1 Fe2 FIZZLED ID: 173595

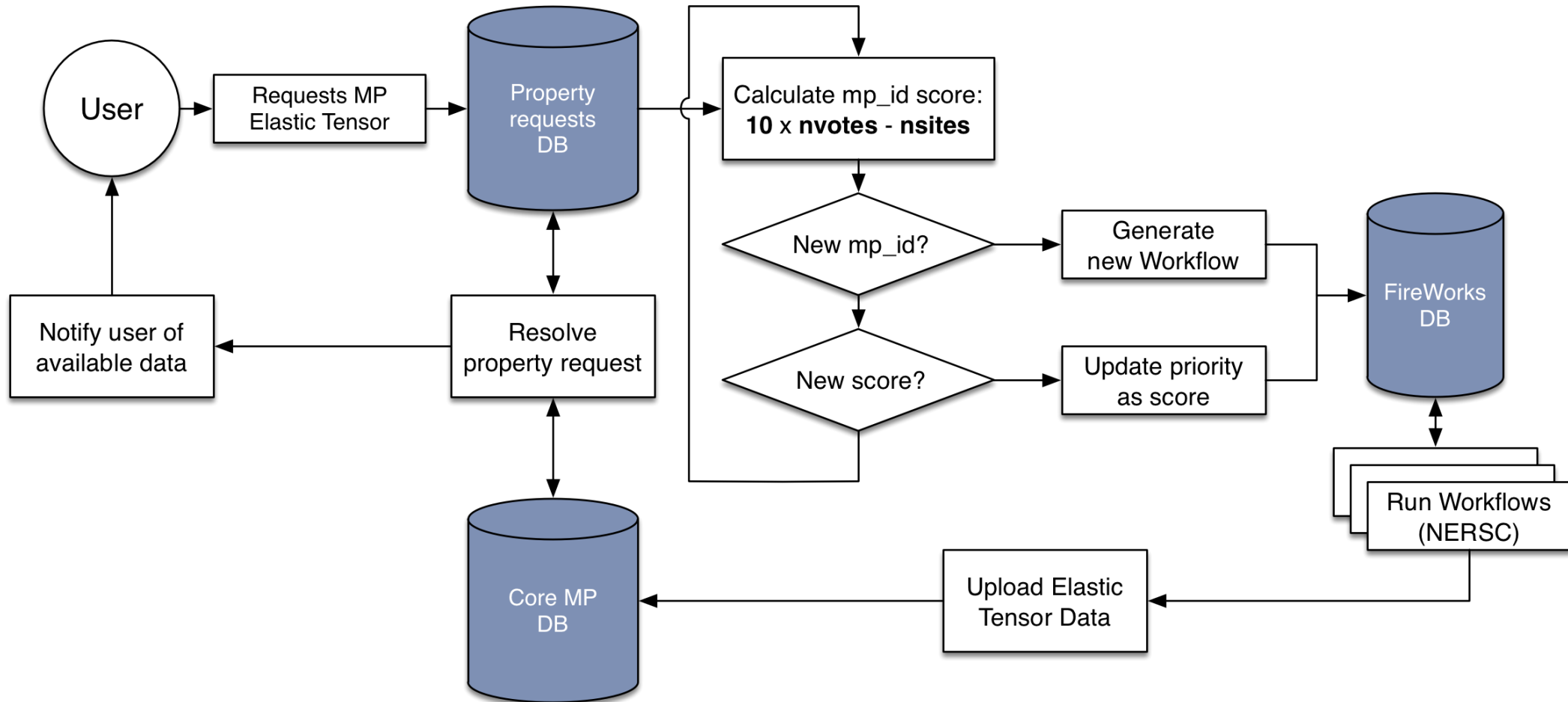
- Al1\_Fe2--VASP\_db\_Insertion
- Al1\_Fe2--Optimize\_deformed\_structure
- Al1\_Fe2--Add\_Deformed\_Struct\_to\_SNL\_database
- Al1\_Fe2--VASP\_db\_Insertion

**Current Database Status**

	Fireworks	Workflows
<span>RUNNING</span>	247	272
<span>ARCHIVED</span>	0	0
<span>WAITING</span>	13,948	0
<span>FIZZLED</span>	811	64
<span>READY</span>	5,668	1,806
<span>RESERVED</span>	7	0
<span>COMPLETED</span>	151,377	1,659
<span>DEFUSED</span>	1,482	46
<b>TOTAL</b>	<b>173,540</b>	<b>3,847</b>

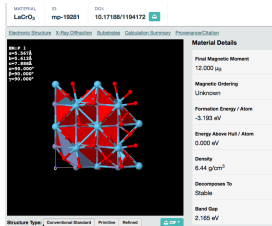


# Priorities of elastic tensor workflows can be dynamically updated





# All together now



material  
detail



workflow  
detail

filter:  , sort:  incr  decr votes:  incr  decr

Show only what I have upvoted

ID	description	votes	E above hull / atom (eV)	detail
<a href="#">mp-19281</a>	LaCrO <sub>3</sub> Pnam	3	0	N/A
<a href="#">mp-5929</a>	Na <sub>5</sub> SiP <sub>3</sub> P2 <sub>1</sub> /c	1	0	<a href="#">workflow</a>
<a href="#">mp-780628</a>	Li <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub> C2/c	0	0.050	N/A
<a href="#">mp-1960</a>	Li <sub>2</sub> O Fm $\bar{3}$ m	N/A	0	<a href="#">tensor</a>



property  
detail

Elasticity

Reference for tensor and properties:  Visualize with ELATE

Stiffness Tensor C <sub>ij</sub> (GPa)					
196.75	18.82	18.77	0	0	0
18.82	196.84	18.82	0	0	0
18.77	18.82	196.76	0	0	0
0	0	0	59.15	0	0
0	0	0	0	59.15	0
0	0	0	0	0	59.15

Shear Modulus G <sub>y</sub>	Bulk Modulus K <sub>v</sub>
71.08 GPa	78.13 GPa
Shear Modulus G <sub>11</sub>	Bulk Modulus K <sub>s</sub>
68.31 GPa	78.13 GPa
Shear Modulus G <sub>v11</sub>	Bulk Modulus K <sub>v11</sub>
69.70 GPa	78.13 GPa
Elastic Anisotropy	Poisson's Ratio
0.20	0.16

# One main endpoint, with ample options

/rows?format=html&filter=W-\*&psort=decr&ssort=incr&psize=5

## Interactive Leaderboard for Property Requests and Notification

Logged in as maartendft@gmail.com






[Log out](#)

filter:  , sort:  incr  decr votes,  incr  decr E above hull / atom (eV)

Show only what I have upvoted

Go

[reset all](#)

ID	description	votes	E above hull / atom (eV)	detail
<a href="#">mp-1821</a>	WSe <sub>2</sub> P6 <sub>3</sub> /mmc	5 	0	<a href="#">workflow</a>
<a href="#">mp-224</a>	WS <sub>2</sub> P6 <sub>3</sub> /mmc	2 	0	<a href="#">workflow</a>
<a href="#">mp-30336</a>	Al <sub>4</sub> W Cm	1 	0.0001491496	<a href="#">workflow</a>
<a href="#">mp-12524</a>	Al <sub>2</sub> W P6 <sub>4</sub> 22	1 	0.0963289224444	<a href="#">workflow</a>
<a href="#">mp-979289</a>	TaW <sub>3</sub> Fm $\bar{3}$ m	0 	0	N/A

[Next →](#)

# Configuration is mostly data, some functions

## entries

```
import pymongo
from pymatgen import MPRester

def describe_entry(e, fields):
    """Join fields in entry e to provide a string description.

    Example:
    >>> e = {'formula': 'LiCoO2', 'spacegroup': {'symbol': 'R-3m'}}
    >>> describe_entry(e, ['formula', 'spacegroup.symbol'])
    'LiCoO2 R-3m'
    """
    from operator import getitem
    return " ".join([reduce(getitem, f.split('.'), e)
                     for f in fields])

def describe_entry_html(description):
    import re
    formula, spacegroup = description.split(" ")
    formula = re.sub(r'\s', r' ', formula)
    formula = re.sub(r'(\.?d+.\d*)', r'<sub>\1</sub>', formula)
    spacegroup = re.sub(r'\(\d)', r'<sub>\1</sub>', spacegroup)
    spacegroup = re.sub(r'\-(\d)',
                       r'<span style="text-decoration:overline;">\1</span>',
                       spacegroup)
    return "{} {}".format(formula, spacegroup)

ENTRIES = {
    'has_property': {
        'elasticity': {'$exists': True}
    },
    'missing_property': {
        'elasticity': {'$exists': False}
    },
    'e_id': 'task_id',
    'extrasort': {
        'field': 'e_above_hull',
        'label': 'E above hull / atom (eV)',
        'default': pymongo.ASCENDING
    },
    'url_for_entry': 'https://materialsproject.org/materials/{e_id}',
    'url_for_prop': 'https://materialsproject.org/materials/{e_id}',
    'description_fields': ['pretty_formula', 'spacegroup.symbol'],
    'describe_entry': describe_entry,
    'describe_entry_html': describe_entry_html,
    'filter': {
        'placeholder': 'Fe-0',
        'transform': MPRester.parse_criteria
    },
    'filter_fields': ['elasticity.K_VRH', 'chemsys'],
    'rows_per_page': 10,
}
```

## workflows

```
def get_workflow_ids(entry_ids, workflow_collection):
    fireworks = workflow_collection.database.fireworks
    fk_field = "spec.snلabout_mp_id"
    fws = fireworks.find({'fk_field': {'$in': entry_ids},
                          {'_id': 0, "fw_id": 1, fk_field: 1}})

    idmap = {}
    for fw in fws:
        entry_id = fw['spec']['snل']['about']['_mp_id']
        idmap[entry_id] = fw['fw_id']
    return [idmap.get(e_id, None) for e_id in entry_ids]

WORKFLOWS = {
    'get_workflow_ids': get_workflow_ids,
    'url_for': 'http://elastic.dash.materialsproject.org/wf/{w_id}',
}
```

## db connections

```
USE_TEST_CLIENTS = True
CLIENTS = {
    'votes': {
        'host': 'host1',
        'port': 27017,
        'database': 'mg_apps_prod',
        'collection': 'property_requests',
        'username': 'ilprn_readwrite',
        'password': 'pass',
    },
    'entries': {
        'host': 'host2',
        'port': 27017,
        'database': 'mg_core_prod',
        'collection': 'materials',
        'username': 'ilprn_readonly',
        'password': 'pass',
    },
    'workflows': {
        'host': 'host3',
        'port': 27017,
        'database': 'fw_ilm_elastic',
        'collection': 'workflows',
        'username': 'ilprn_readonly',
        'password': 'pass',
    }
}
```

## votes

```
def user_voted(email, prefilter=True, votes_doc=None):
    if prefilter:
        return {'requesters': email}
    else:
        return email in votes_doc['requesters']

def record_vote(email, votes_doc, votes_collection, how, filt_for_update):
    assert how in ['up', 'down']
    if how == 'up':
        assert email not in votes_doc.get('requesters', [])
    else:
        assert email in votes_doc['requesters']

    op = '$push' if how == 'up' else '$pull'
    amt = 1 if how == 'up' else -1
    update = {'$inc': {'nrequesters': amt}, op: {'requesters': email}}
    votes_collection.update_one(filt_for_update, update, upsert=True)
    return "success: {}voted {}".format(how, filt_for_update['material_id'])

VOTES = {
    'filter_active': {'state': {'$ne': 'COMPLETED'}, 'prop': 'elasticity'},
    'filter_completed': {'state': 'COMPLETED', 'prop': 'elasticity'},
    'entry_id': 'material_id',
    'prop_field': 'prop',
    'prop_value': 'elasticity',
    'requesters': 'requesters',
    'nvotes': 'nrequesters',
    'user_voted': 'user_voted',
    'record_vote': 'record_vote',
    'projection_extras': ['requesters'],
    'max_active_votes_per_user': 10,
}
```

## token-based auth

```
PASSWORDLESS = {
    'TOKEN_STORE': 'mongo',
    'DELIVERY_METHOD': 'null',
    'LOGIN_URL': 'plain',
    'dbname': 'ilprn_test',
    'remote_app_id': 'materialsproject.org',
    'remote_app_secret': 'SECRET',
    'remote_app_name': 'Materials Project',
    'remote_app_uri': 'https://materialsproject.org',
}
```

# Remaining Work

- Merge existing email notification service with leaderboard codebase
- Deploy leaderboard with auth via dynamically fetched token link
  - on Materials Project user dashboard
  - at “point-of-sale” (e.g. on request of property prediction)
- Communicating expectations
  - “special” users / community expectations on vote (re)weighting
  - troubleshooting failed “user” workflows
- Release codebase and documentation
  - Will be under [github.com/materialsproject](https://github.com/materialsproject)
  - In the meantime, contact me: [dwinston@lbl.gov](mailto:dwinston@lbl.gov)