

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

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A database of inorganic crystalline material structures and properties

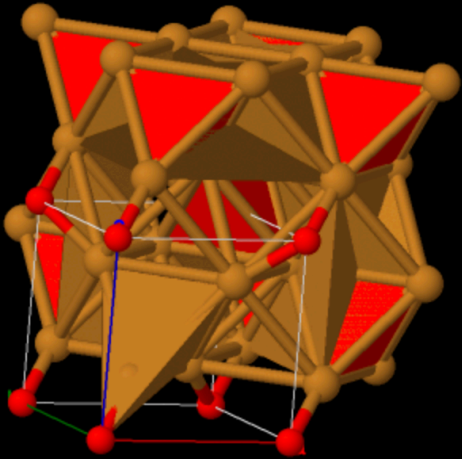
MATERIAL
Cu₂O

ID:
mp-361

DOI:
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_B

Magnetic Ordering
Unknown


Formation Energy / Atom
-0.650 eV

Energy Above Hull / Atom
0.000 eV

Density
6.03 g/cm³


Decomposes To
Stable

Band Gap
0.500 eV

Reference for tensor and properties: 

Stiffness Tensor C_{ij} (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_{ij}

Visualize with ELATE 


Shear Modulus G_V 8.40 GPa	Bulk Modulus K_V 111.57 GPa
Shear Modulus G_R 8.31 GPa	Bulk Modulus K_R 111.57 GPa
Shear Modulus G_{VRH} 8.35 GPa	Bulk Modulus K_{VRH} 111.57 GPa
Elastic Anisotropy 0.05	Poisson's Ratio 0.46

Structure Type:

Conventional Standard

Primitive

Refined

 CIF

<https://www.materialsproject.org>

1

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

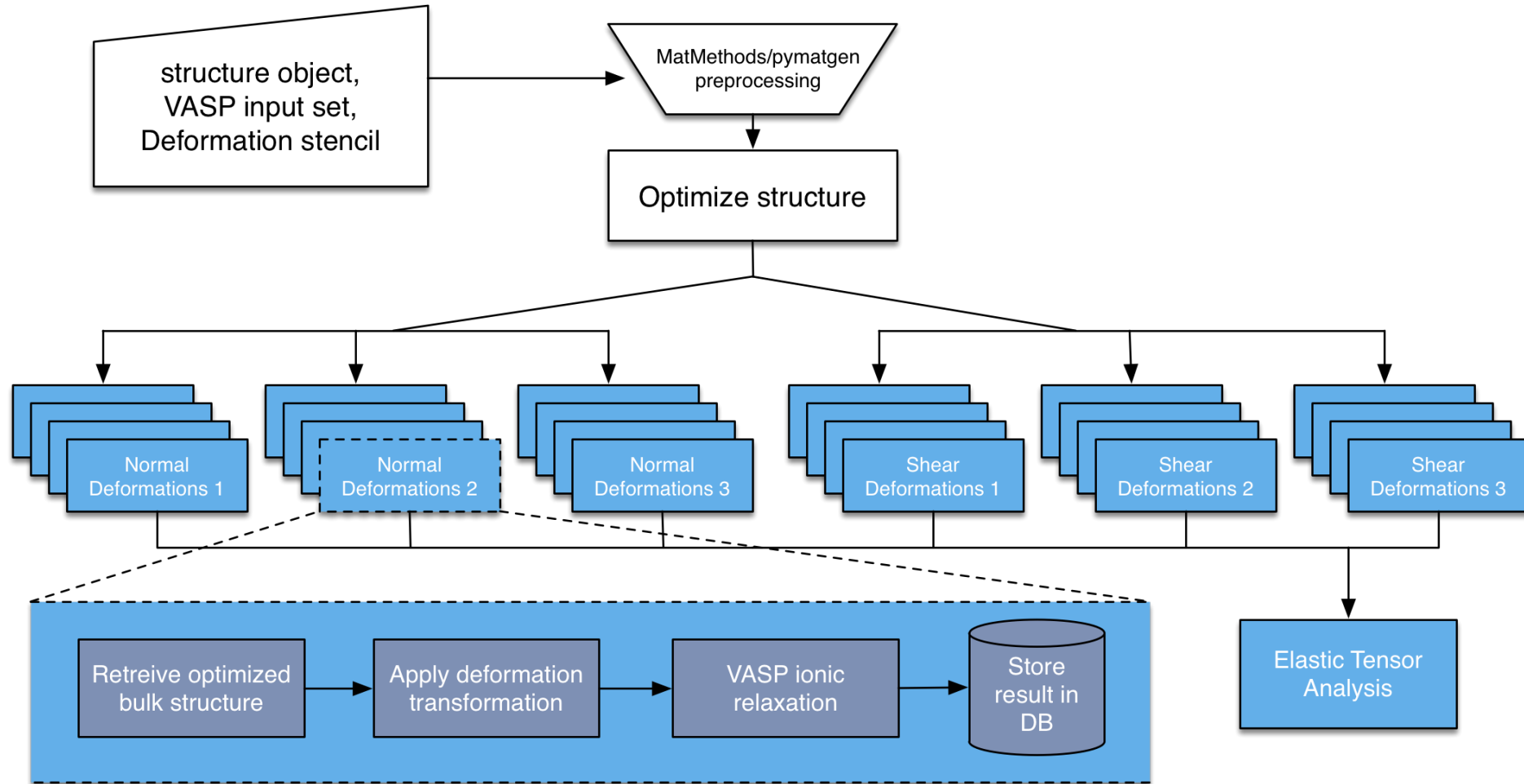
3,628

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}

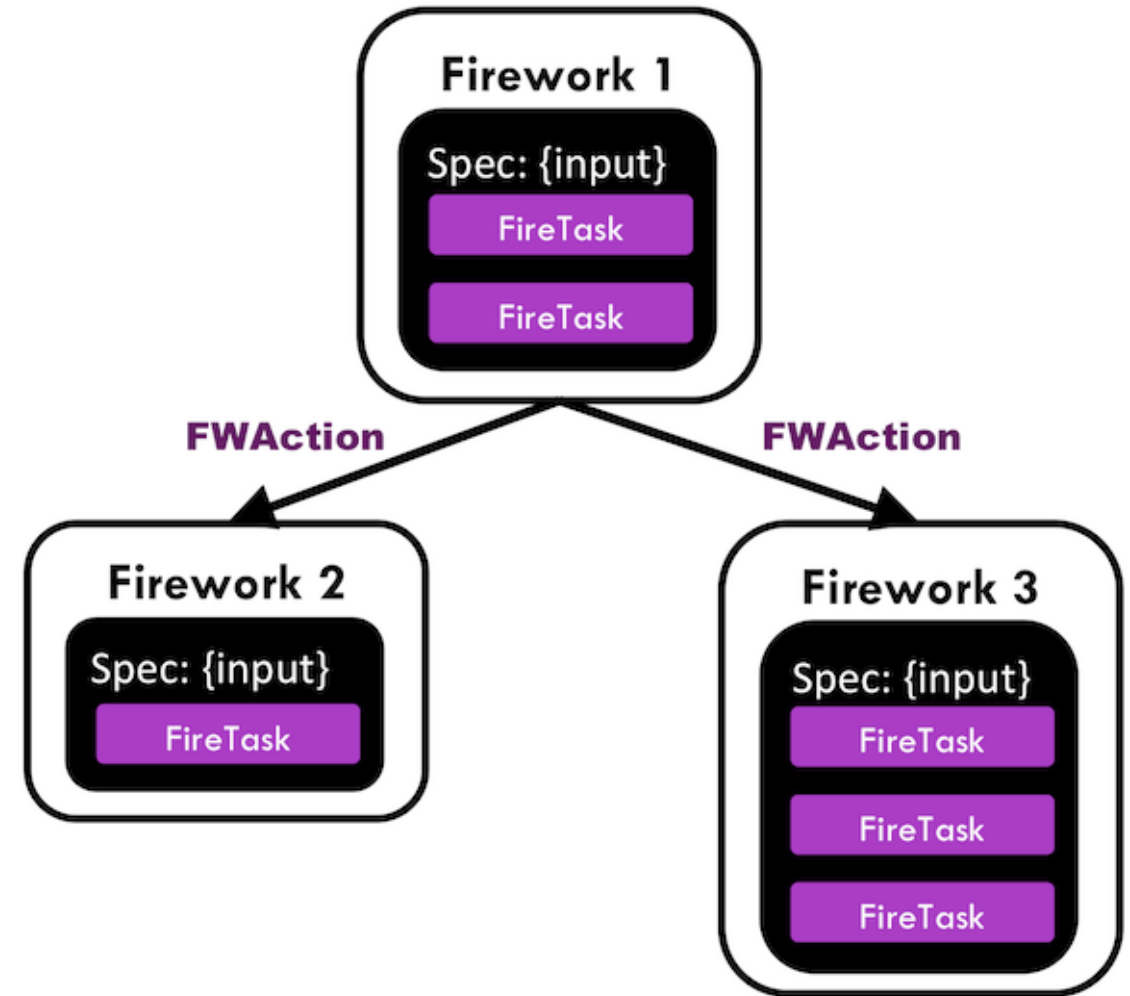
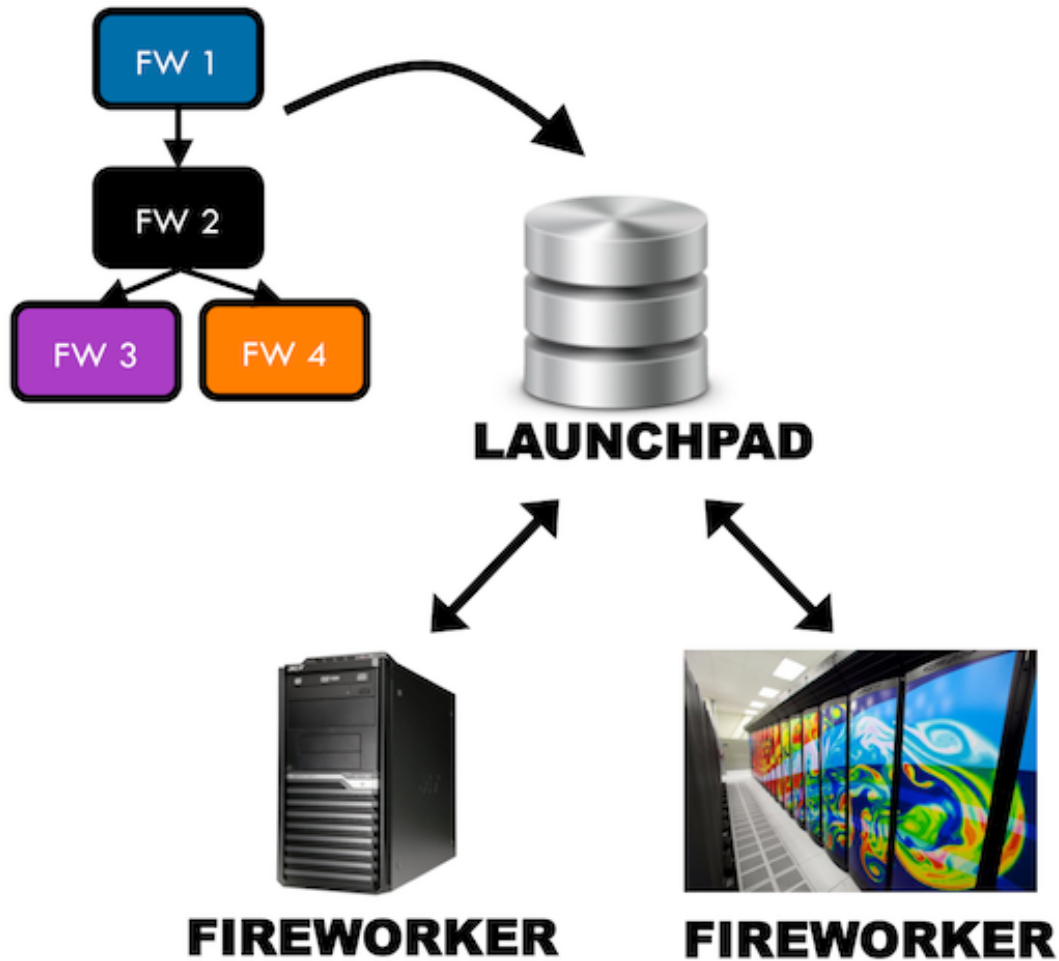
76.12 GPa

ⓘ **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

FireWorks

Workflow Dashboard

Newest Workflows

Cr1 Si1 Te3 READY ID: 173672

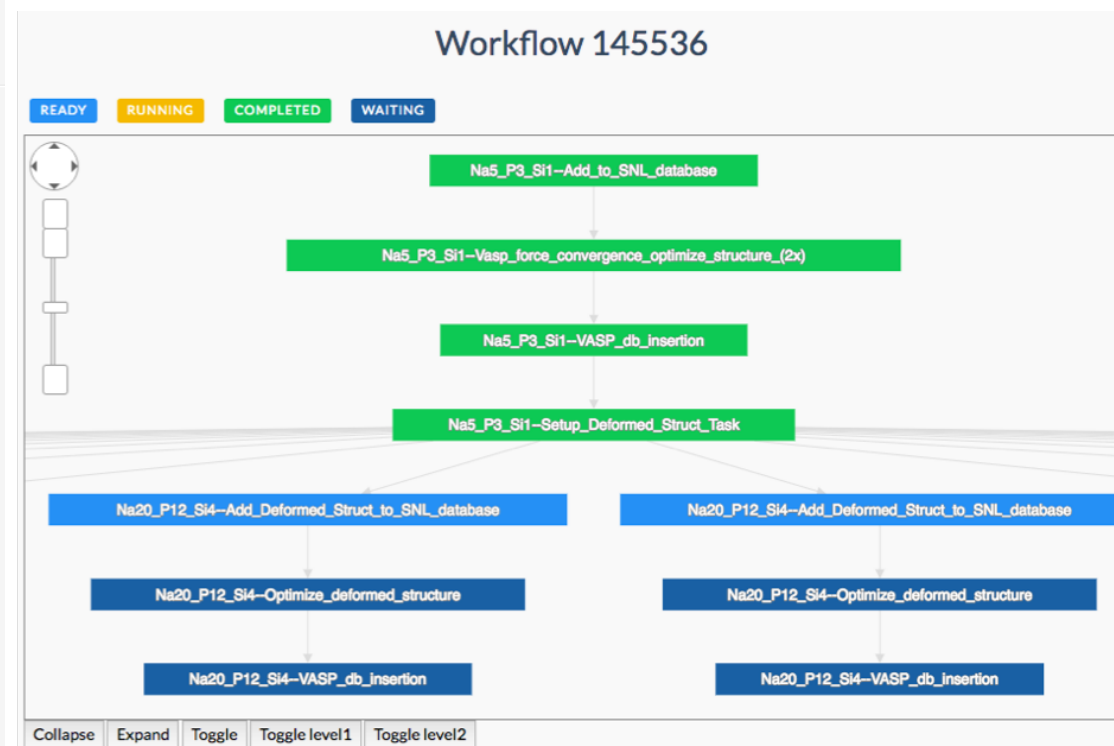
- Cr1_Si1_Te3--Setup_Deformed_Struct_Task
- Cr1_Si1_Te3--VASP_db_Insertion
- Cr1_Si1_Te3--Vasp_force_convergence_optimize_structure_(2x)
- Cr1_Si1_Te3--Add_to_SNL_database

Al1 Fe2 FIZZLED ID: 173595

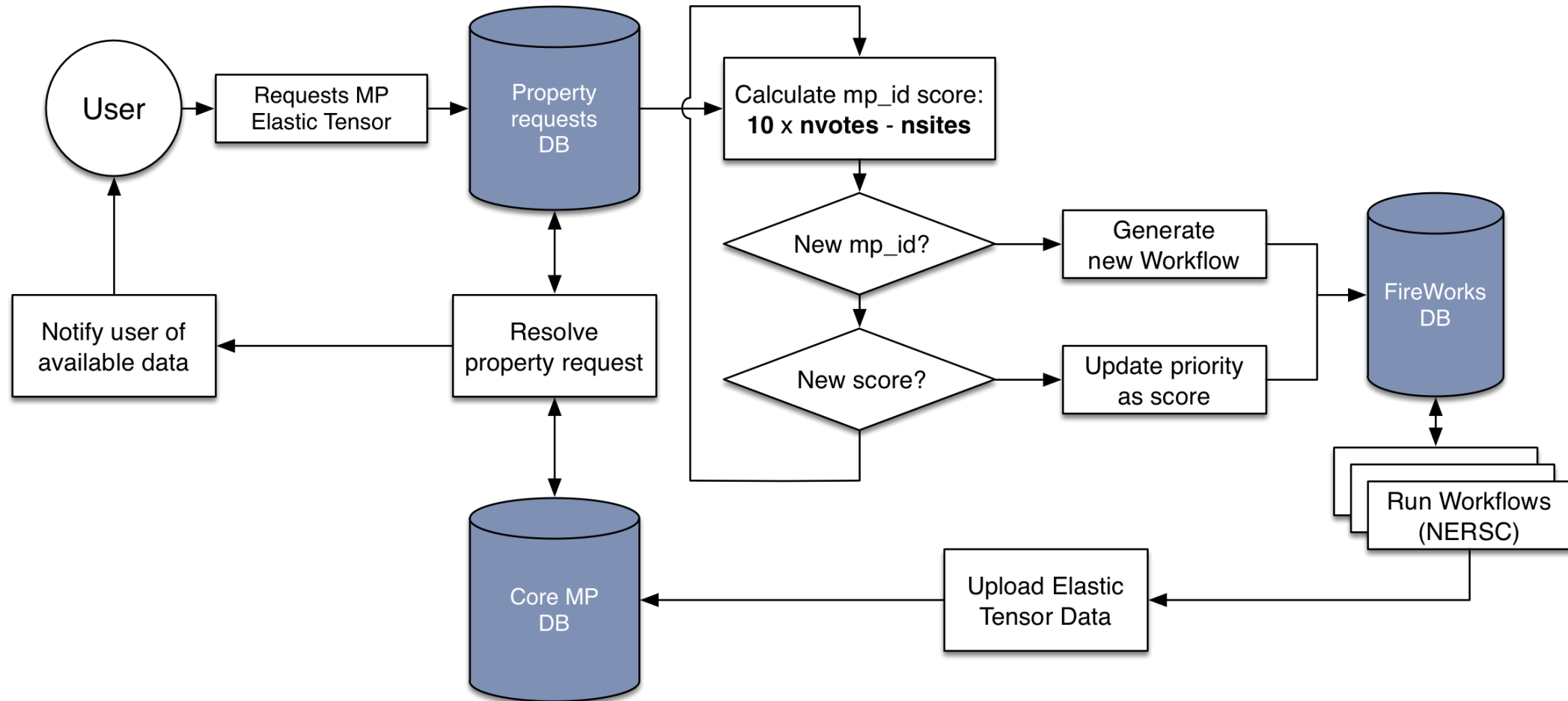
- Al1_Fe2--VASP_db_Insertion
- Al1_Fe2--Optimize_deformed_structure
- Al1_Fe2--Add_Deformed_Struct_to_SNL_database
- Al1_Fe2--VASP_db_Insertion

Current Database Status

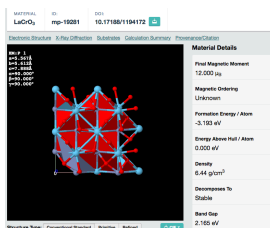
	Fireworks	Workflows
RUNNING	247	272
ARCHIVED	0	0
WAITING	13,948	0
FIZZLED	811	64
READY	5,668	1,806
RESERVED	7	0
COMPLETED	151,377	1,659
DEFUSED	1,482	46
TOTAL	173,540	3,847



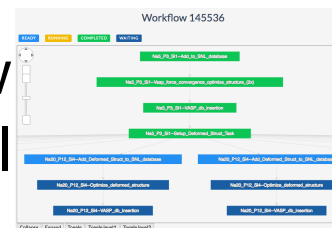
Priorities of elastic tensor workflows can be dynamically updated



All together now



material
detail



workflow
detail

filter: , sort: ☐ incr ☒ decr votes: ☒ incr ☐ decr

☐ Show only what I have upvoted

E above hull / atom (eV)

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

property
detail

Elasticity

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

Stiffness Tensor C _{ij} (GPa)						Shear Modulus G _V	Bulk Modulus K _V
196.75	18.82	18.77	0	0	0	71.08 GPa	78.13 GPa
18.82	196.84	18.82	0	0	0	78.13 GPa	68.31 GPa
18.77	18.82	196.76	0	0	0	68.31 GPa	78.13 GPa
0	0	0	59.15	0	0	69.70 GPa	78.13 GPa
0	0	0	0	59.15	0	69.70 GPa	78.13 GPa
0	0	0	0	0	59.15	69.70 GPa	78.13 GPa
0	0	0	0	0	0	69.70 GPa	78.13 GPa
Compliance Tensor S _{ij}						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 [reset all](#)

ID	description	votes	E above hull / atom (eV)	detail
mp-1821	WSe ₂ P6 ₃ /mmc	5 	0	workflow
mp-224	WS ₂ P6 ₃ /mmc	2 	0	workflow
mp-30336	Al ₄ W Cm	1 	0.0001491496	workflow
mp-12524	Al ₂ W P6 ₄ 22	1 	0.0963289224444	workflow
mp-979289	TaW ₃ 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'<sub>\1</sub>', spacegroup)
    r'<span style="text-decoration:underline;">\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}',
}
```

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,
}
```

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',
    }
}
```

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
 - In the meantime, contact me: dwinston@lbl.gov
- *Update: code online at <https://github.com/materialsproject/ilprn>*