## 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

Cu <sub>2</sub> O	iD: <b>mp-361</b>	10.17188/1207131											
HM:P 1			Material Details										
a=4.288Å b=4.288Å c=4.288Å α=90.000° β=90.000°			Final Magnetic Moment 0.000 µ <sub>B</sub>	Final Magnetic Moment         0.000 μ <sub>B</sub>								Visualize with ELATE	
γ=90.000°			Magnetic Ordering		Stiffness Tensor Cij (GPa)						Shear Modulus G <sub>V</sub>	Bulk Modulus K <sub>V</sub>	
			Unknown		124.16	105.26	105.27	0	0	0	8.40 GPa	111.57 GPa	
			Formation Energy / Atom		105.26	124.17	105.27	0	0	0	Shear Modulus G <sub>R</sub>	Bulk Modulus K <sub>R</sub>	
			-0.050 EV		105.27	105.27	124.18	0	0	0	8.31 GPa	111.57 GPa	
			Energy Above Hull / Atom 0.000 eV		0	0	0	7.69	0	0	Shear Modulus G <sub>VRH</sub>	Bulk Modulus K <sub>VRH</sub>	
			Donaity		0	0	0	0	7.69	0	8.35 GPa	111.57 GPa	
			6.03 g/cm <sup>3</sup>		0	0	0	0	0	7.69	Elastic Anisotropy	Poisson's Ratio	
			Decomposes To		Compliance Tensor Sij						0.05	0.46	
			Stable										
			Band Gap										
Structure Type:	Conventional St	andard Primitive Refined	0.500 eV			-							

#### https://www.materialsproject.org

## Some calculated properties are useful but computationally expensive



## 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:



doi:10.1038/srep34256 https://github.com/materialsproject/gbml



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



https://github.com/materialsproject/fireworks

## FireWorks has built-in web-based monitoring



## Priorities of elastic tensor workflows can be dynamically updated



## All together now







## One main endpoint, with ample options

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

#### Logged in as maartendft@gmail.com Interactive Leaderboard for Property **Requests and Notification**

🔿 incr o incr W-\* sort: filter: E above hull / atom (eV) votes, 💿 decr decr Show only what I have upvoted reset all Go E above hull / ID description atom (eV) detail votes 5 × mp-1821 WSe<sub>2</sub> P6<sub>3</sub>/mmc 0 workflow 2 mp-224 WS<sub>2</sub> P6<sub>3</sub>/mmc 0 workflow 1 X mp-30336 Al₄W Cm 0.0001491496 workflow 1 X mp-12524 Al<sub>2</sub>W P6<sub>4</sub>22 0.0963289224444 workflow 0  $TaW_3 Fm\overline{3}m$ mp-979289 0 N/A

Log out

## Configuration is mostly data, some functions

#### entries



#### workflows

<pre>get_workflow_ids(entry_ids, workflow_collection): fireworks = workflow_collection.database.fireworks fk_field = "spec.snl.aboutmp_id" fws = fireworks.find({fk_field: {"\$in": entry_ids}}, {"_id": 0, "fw_id": 1, fk_field: 1})</pre>
idmap = {}
for fw in fws:
<pre>entry_id = fw['spec']['snl']['about']['_mp_id'] idmap[entry_id] = fw['fw_id'] return [idmap.get(e_id, None) for e_id in entry_ids]</pre>
<pre>KFLOWS = {     'get_workflow_ids,     'url_for': 'http://elastic.dash.materialsproject.org/wf/{w_id}'</pre>

def user voted(email, prefilter=True, votes doc=None): def record\_vote(email, votes\_doc, votes\_collection, how, filt\_for\_update):

assert email not in votes\_doc.get('requesters', [])

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'])

'filter\_active': {'state': {'\$ne': 'COMPLETED'}, 'prop': 'elasticity'}, 'filter\_completed': {'state': 'COMPLETED', 'prop': 'elasticity'}, 'entry\_id': 'material\_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',

> 'host': 'host2', 'port': 27017, 'database': 'mg\_core\_prod', 'collection': 'materials', 'username': '<u>ilprn readonly</u>', 'password': 'pass',

'workflows': { 'host': 'host3', 'port': 27017, 'database': '<u>fw jhm</u>elastic', 'collection': 'workflows',
'username': 'ilprn\_readonly', 'password': 'pass',

#### token-based auth

#### ASSWORDLESS = $\{$

'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: <u>dwinston@lbl.gov</u>
- Update: code online at <a href="https://github.com/materialsproject/ilprn">https://github.com/materialsproject/ilprn</a>