



***TRUST*: Team for Research in Ubiquitous Secure Technology**

FireWorks and the Materials Project: Facilitating Scientific Workflows

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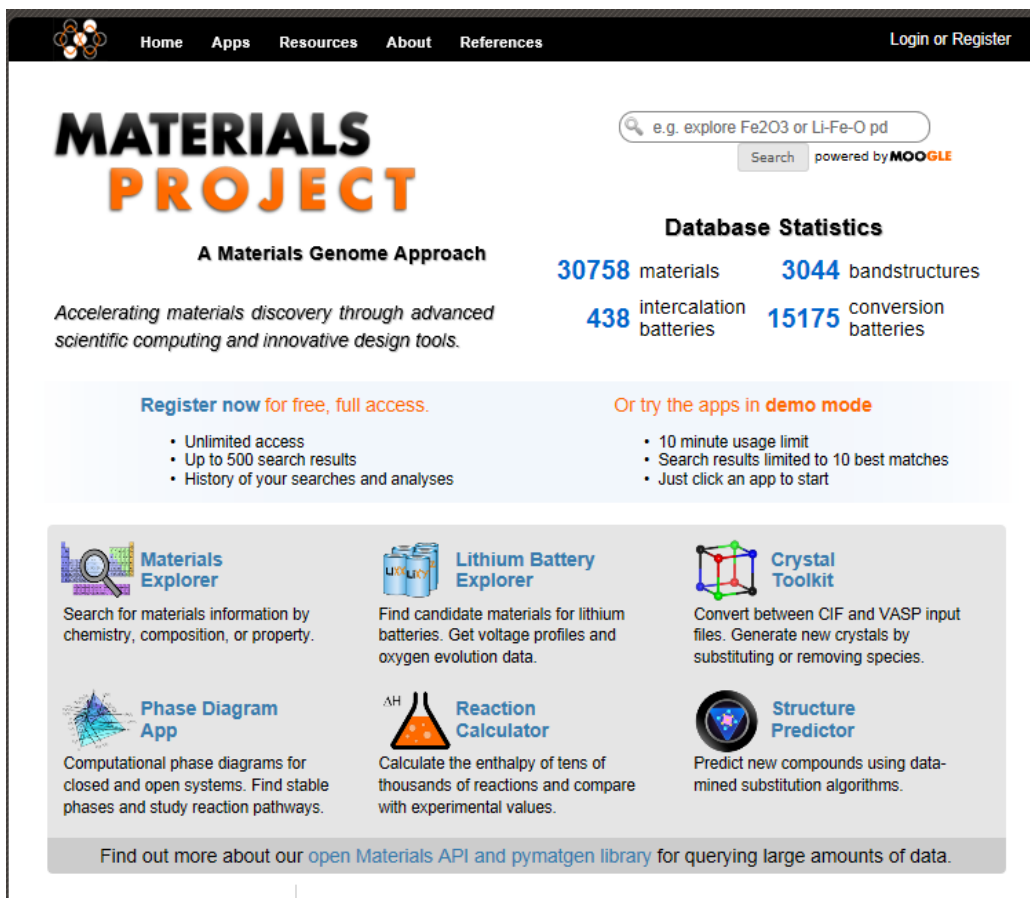
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The Materials Project

The Materials Project aims to accelerate materials innovation and design by providing free access to a searchable, interactive database of computed materials properties spanning most known inorganic compounds.



The screenshot shows the Materials Project website interface. At the top is a navigation bar with links: Home, Apps, Resources, About, References, and a Login or Register button. Below the navigation bar is a large search bar with the placeholder text "e.g. explore Fe₂O₃ or Li-Fe-O pd" and a "Search" button. To the right of the search bar, it says "powered by MOOGL".

The main content area features the "MATERIALS PROJECT" logo in large, bold letters. Below the logo is the tagline "A Materials Genome Approach" and a description: "Accelerating materials discovery through advanced scientific computing and innovative design tools."

To the right of the logo, there is a "Database Statistics" section with the following data:

Category	Count
materials	30758
bandstructures	3044
intercalation batteries	438
conversion batteries	15175

Below the statistics, there are two sections: "Register now for free, full access." and "Or try the apps in demo mode".

The "Register now for free, full access." section lists the following benefits:

- Unlimited access
- Up to 500 search results
- History of your searches and analyses

The "Or try the apps in demo mode" section lists the following limitations:

- 10 minute usage limit
- Search results limited to 10 best matches
- Just click an app to start

Below these sections, there is a grid of six application tiles, each with an icon, a title, and a brief description:

- Materials Explorer**: Search for materials information by chemistry, composition, or property.
- Lithium Battery Explorer**: Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.
- Crystal Toolkit**: Convert between CIF and VASP input files. Generate new crystals by substituting or removing species.
- Phase Diagram App**: Computational phase diagrams for closed and open systems. Find stable phases and study reaction pathways.
- Reaction Calculator**: Calculate the enthalpy of tens of thousands of reactions and compare with experimental values.
- Structure Predictor**: Predict new compounds using data-mined substitution algorithms.

At the bottom of the page, there is a footer that says: "Find out more about our [open Materials API](#) and [pymatgen library](#) for querying large amounts of data."



- is a code for defining, managing, and executing scientific workflows
- can be used to automate most types of calculations over arbitrary computing resources, including those that have a queuing system
- is intended to be a friendly workflow software that is easy to get started with but flexible enough to handle complicated use cases

FireWorks is an open source project; documentation and installation instructions can be found at <http://pythonhosted.org/FireWorks>.

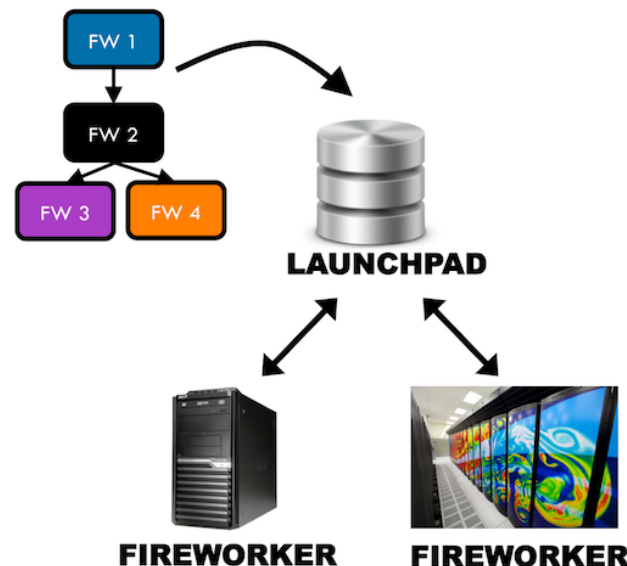
Main Components

LaunchPad

- Manages workflows
 - Can add, query the state of, or rerun workflows

FireWorkers

- Run jobs
 - Request workflows from the LaunchPad, execute them, and send back information



Workflow Model

FireTask

- An atomic computing job
 - Can call a shell script or execute a single Python function

FireWork

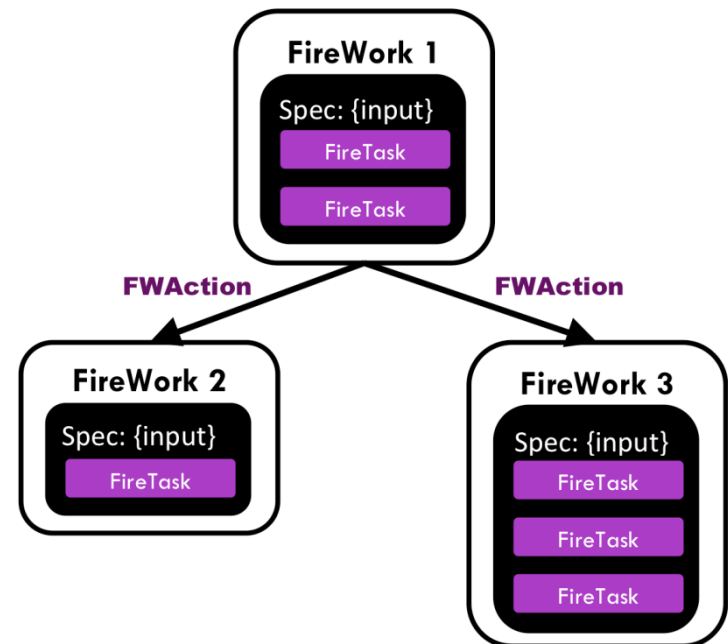
- Contains all information needed to run a job
 - Formatted as a JSON specification, or “spec”

Workflow

- A set of FireWorks
 - FireWorks have dependencies between them

FWAction

- Can be returned between FireWorks
 - Can store data or modify the workflow depending on the output





Materials Project Workflow Dashboard

257,133 Completed FireWorks as of 2013-08-01, 12:06 (PDT)

Recent Activity

Newest Fireworks		
ID	Name	State
376175	O2_Si1--VASP_db_insertion	WAITING
376174	O2_Si1--GGA_static	READY
376173	O2_Si1--VASP_db_insertion	WAITING
376172	O2_Si1--GGA_band_structure_v2	WAITING
376170	O2_Si1--VASP_db_insertion	WAITING
376168	O2_Si1--GGA_Uniform_v2	WAITING
376166	O2_Si1--VASP_db_insertion	READY
376164	O2_Si1--GGA_static_v2	FIZZLED
376171	O2_Si1--VASP_db_insertion	WAITING

Current Database Status		
	Fireworks	Workflows
ARCHIVED	110079	23189
DEFUSED	5283	2501
WAITING	2534	
READY	765	612
RESERVED	2	
FIZZLED	359	138
RUNNING	19	78
COMPLETED	257133	64658
TOTAL	376174	91176

Newest Workflows		
ID	Name	State
376099	O2 Si1	FIZZLED
376066	O2 Si1	FIZZLED
376097	O2 Si1	FIZZLED
376096	O2 Si1	FIZZLED
374102	O2 Si1	FIZZLED
376078	O2 Si1	FIZZLED
376072	O2 Si1	RUNNING
375618	O2 Si1	RUNNING
371904	O2 Si1	RUNNING

[Home](#) | [Fireworks Index](#) | [Workflows Index](#) | [Testing](#)

© Copyright 2013, [FireWorks](#).

376174 Fireworks currently in database

[NEWEST](#) | [ARCHIVED](#) | [DEFUSED](#) | [WAITING](#) | [READY](#) | [RESERVED](#) | [FIZZLED](#) | [RUNNING](#) | [COMPLETED](#)

Click an ID for more information about that Firework.

Newest Fireworks

ID	Name	State
376175	O2_Si1--VASP_db_insertion	WAITING
376174	O2_Si1--GGA_static	READY
376173	O2_Si1--VASP_db_insertion	WAITING
376172	O2_Si1--GGA_band_structure_v2	WAITING
376170	O2_Si1--VASP_db_insertion	WAITING
376168	O2_Si1--GGA_Uniform_v2	WAITING
376166	O2_Si1--VASP_db_insertion	READY
376164	O2_Si1--GGA_static_v2	FIZZLED
376171	O2_Si1--VASP_db_insertion	WAITING
376169	O2_Si1--GGA_band_structure_v2	WAITING

1 of 37618 > >>

138 Fizzled Workflows currently in database

[NEWEST](#) | [ARCHIVED](#) | [DEFUSED](#) | [READY](#) | [FIZZLED](#) | [RUNNING](#) | [COMPLETED](#)

Click an ID for more information about that Workflow.

Fizzled Workflows

ID	Name
362280	Be1 Na2 O6 Si2
361552	Pd3 Rb2 Se4
156491	Cl1 S1
360320	Mn2 Na2 S3
359364	O4 Pb2 Sn1
359673	O3 Sm2
357643	O2 Si1
354169	F6 K2 Zr1
340777	Cl1 H5 N2
149024	F6 Hf1 K2

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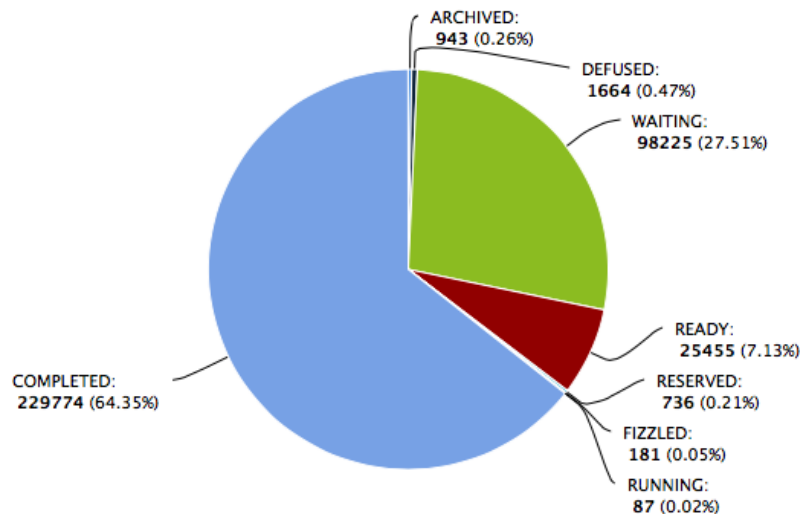
Features (cont.)

Firework 354099 Information

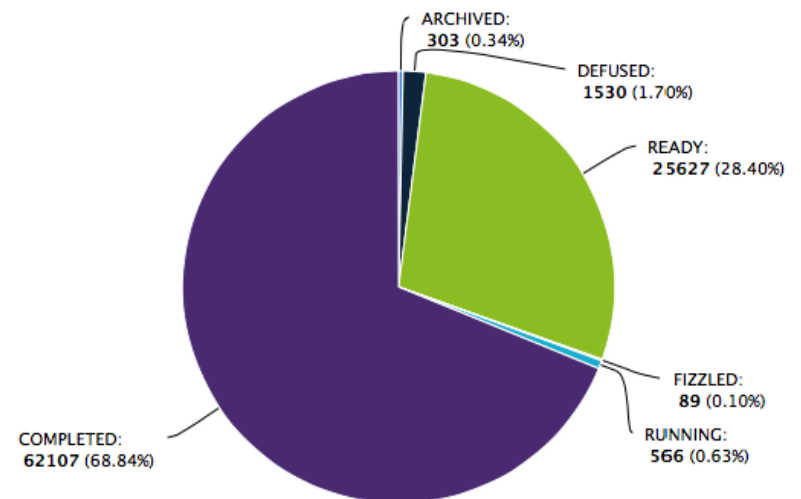
[less](#) | [more](#) | [all](#)

```
{
  "name": "Mg1_O3_Si1--VASP_db_insertion",
  "fw_id": 354099,
  "state": "COMPLETED",
  "created_on": "2013-06-30T10:42:03.523022"
}
```

Current Fireworks Status



Current Workflows Status



Highcharts.com

Acknowledgements

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The Materials Project (www.materialsproject.org)

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Questions?

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FireWorks

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The Materials Project

- www.materialsproject.org
- Email: feedback@materialsproject.org