THE MATERIALS API

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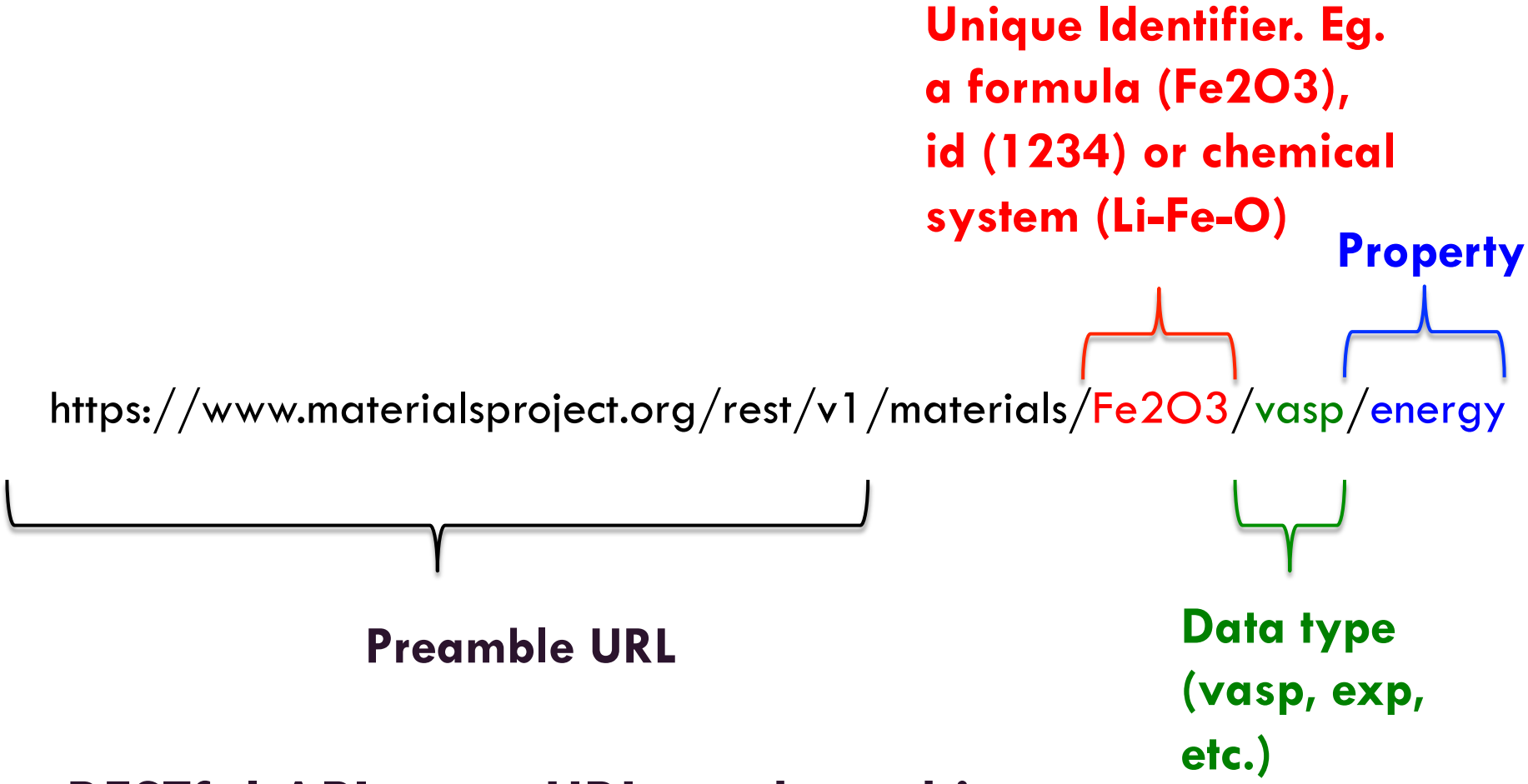
What is The Materials API?

An open platform for accessing Materials Project data based on REpresentational State Transfer (REST) principles.

Flexible and scalable to cater to large number of collaborators, with different access privileges.

Simple to use and code agnostic.

HTTP API design (REST)



- **RESTful API maps URLs to data objects**

Why REST APIs?

- Big push towards RESTful HTTP APIs across the web.
- REST APIs provide programmatic access to data and resources to developers over the web
- Access to data as well defined objects allows users to develop their own custom applications and code

Enables a thriving community built around data.

Access via an API key

- To maintain privileged access, each user has an associated API key (with certain defined access privileges).

- To get your key, login to materialsproject.org and go to www.materialsproject.org/profile

- All MP https requests must supply API key as:
  - A x-api-key header, e.g., {'X-API-KEY': 'MYKEY'}, or
  - As a GET or POST variable, e.g., {'API_KEY': 'MYKEY'}

Sample JSON output

GET https://www.materialsproject.org/rest/v1/materials/Fe2O3/vasp/energy


```
{
    created_at: "2012-08-22T02:35:13.201938",
    valid_response: true,
  - version: {
        pymatgen: "2.0.0",
        db: "2012.07.09",
        rest: "0.5"
    },
  - response: [
      - {
            energy: -1205.36883305,
            material_id: 1456
        },
      - {
            energy: -75.19968867,
            material_id: 19770
        },
      - {
            energy: -66.62512425,
            material_id: 24972
        },
      - {
            energy: -149.4288516,
            material_id: 510080
        }
    ],
    copyright: "Copyright 2012, The Materials Project"
}
```

Integration with pymatgen

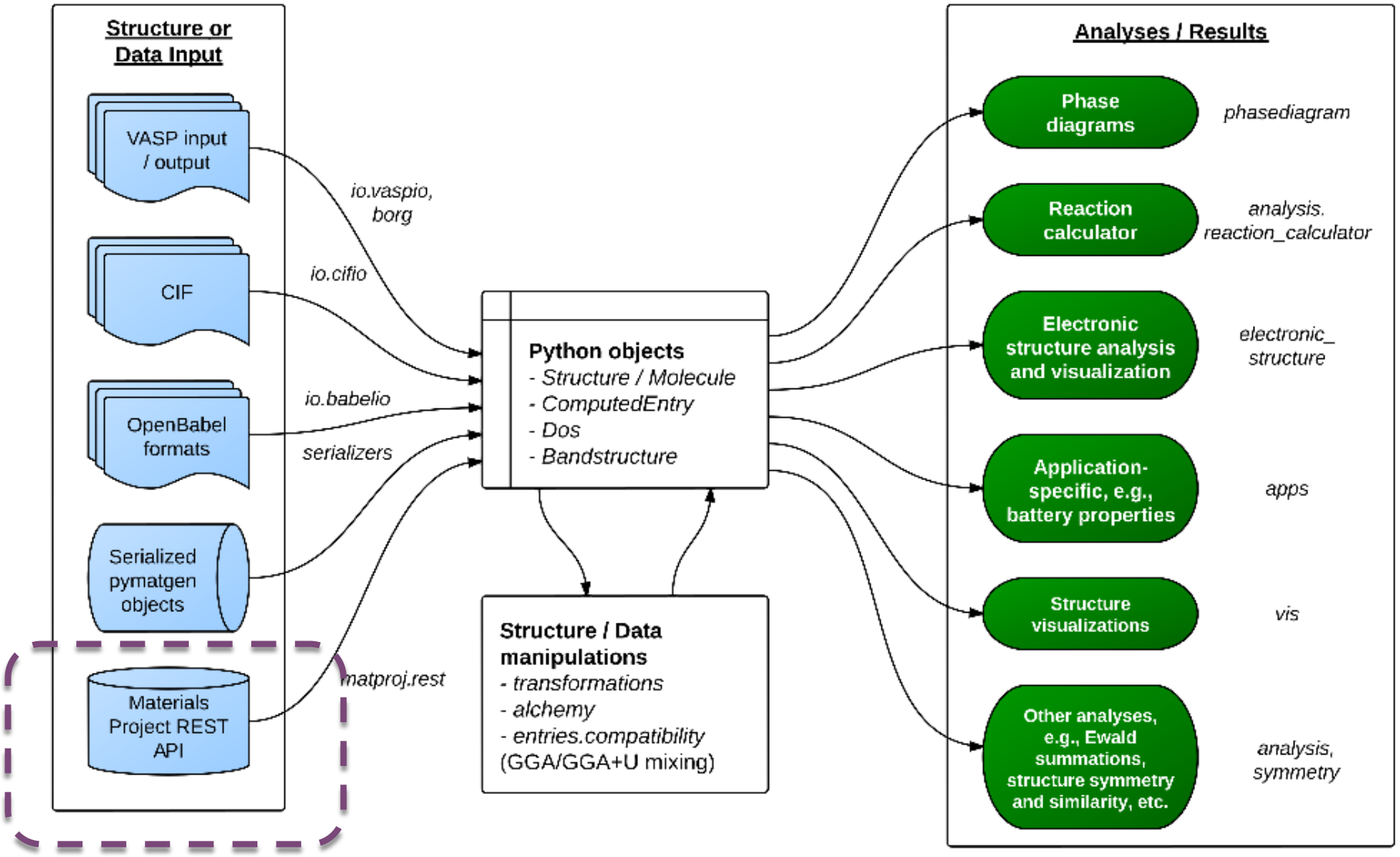
The Materials API

+ pymatgen

Powerful Materials Analytics Tool

pymatgen

- The open source python library that powers the Materials Project.
  - Defines core Python objects for materials data representation.
  - Provides a well-tested set of structure and thermodynamic analysis tools relevant to many applications.
  - Establishes an open platform for researchers to collaboratively develop sophisticated analyses of materials data obtained both from first principles calculations and experiments.



Pymatgen now provides access to analysis functions as well as data

Materials API + pymatgen example

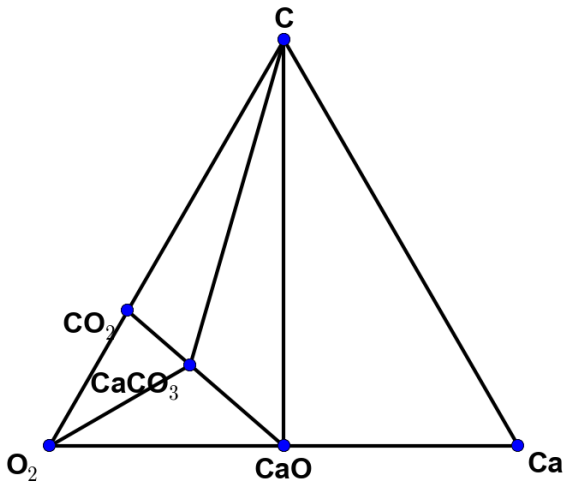
```
from pymatgen.matproj.rest import MPRester

#This initializes the REST adaptor. Put your own API key in.
a = MPRester("YOUR_API_KEY")

#This gives you the Structure corresponding to material id 2254 in the Materials Project.
structure = a.get_structure_by_material_id(2254)

#Entries are the basic unit for thermodynamic and other analyses in pymatgen.
#This gets all entries belonging to the Ca-C-O system.
entries = a.get_entries_in_chemsys(['Ca', 'C', 'O'])

#With entries, you can do many sophisticated analyses,
#like creating phase diagrams.
pd = PhaseDiagram(entries)
plotter = PDPlotter(pd)
plotter.show()
```



More information

- Materials API + pymatgen examples
  - https://gist.github.com/gists/search?q=shyuep+materials+api+pymatgen
- The Materials API wiki
  - https://materialsproject.org/wiki/index.php/The_Materials_API
- Python Materials Genomics
  - http://packages.python.org/pymatgen/
  - Shyue Ping Ong, William Davidson Richard, Anubhav Jain, Geoffroy Hautier, Michael Kocher, Shreyas Cholia, Dan Gunter, Vincent Chevrier, Kristin A. Persson, Gerbrand Ceder. *Python Materials Genomics (pymatgen) : A Robust, Open-Source Python Library for Materials Analysis. (submitted)*