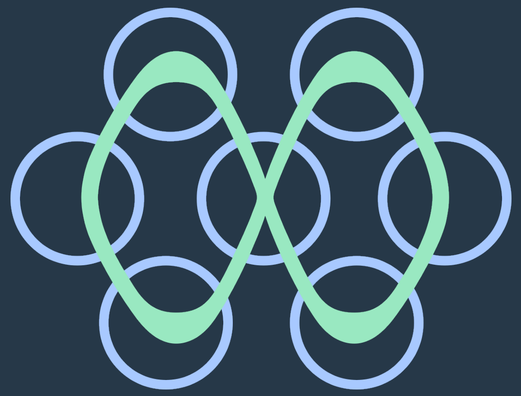
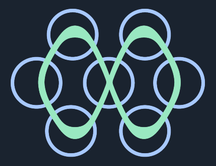


The Materials Project

Workshop 2019



The Materials Project
Workshop 2019

Workshop Overview

Primer Day

1. Technical primer on Python
2. Technical primer on MongoDB

Day 1

1. Introducing the Materials Project, our website and data
2. Introducing pymatgen, our package for crystallographic analysis

Lunch break

3. Case studies on how to use pymatgen to transform crystal structures
4. Accessing MP data with code using pymatgen

Day 2

1. Introducing atomate, our package to help you generate your own data
2. Advanced atomate use

Lunch break

3. Contributing your experimental or computed data to Materials Project
4. Materials Data Science: how to process, analyze and train machine learning models

Feedback and Help

Ask us questions on Slack
mpworkshop.slack.com

Answer exercises during lessons + give feedback: pollev.com/mpworkshop

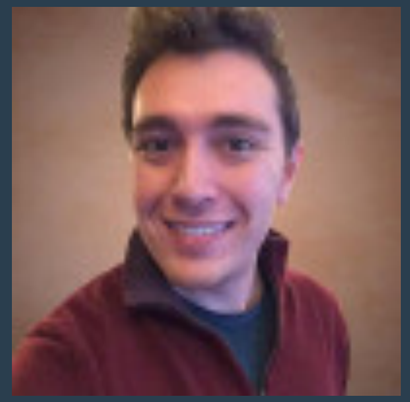
Put up a sticky note on your laptop!
Green is good, red means help

The Materials Project
Workshop 2019

Thursday, 9—10.30am
Introduction to MP data

Instructors:

Donny



John

In this lesson, you will:

- Gain familiarity with the scope of the data the Materials Project offers
- The software we develop to generate this data
- How to access this data via the website
- Introduce how to access this data programmatically with Python

Coffee Break

The Materials Project
Workshop 2019

Thursday, 10.45—12pm
Introduction to pymatgen

Instructors:

Sam

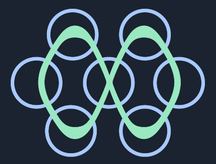
Alex

In this lesson, you will:

- Learn about the essential objects and tools in pymatgen
- Practice using those tools to build, visualize, and manipulate crystal structures and molecules

This lesson's notebook can be found at:

`workshop/pymatgen/1 - pymatgen core use.ipynb`

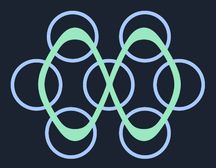


The Materials Project
Workshop 2019

Thursday, 10.45—12pm
Introduction to pymatgen

pymatgen —

The code that powers all scientific analysis in the Materials Project



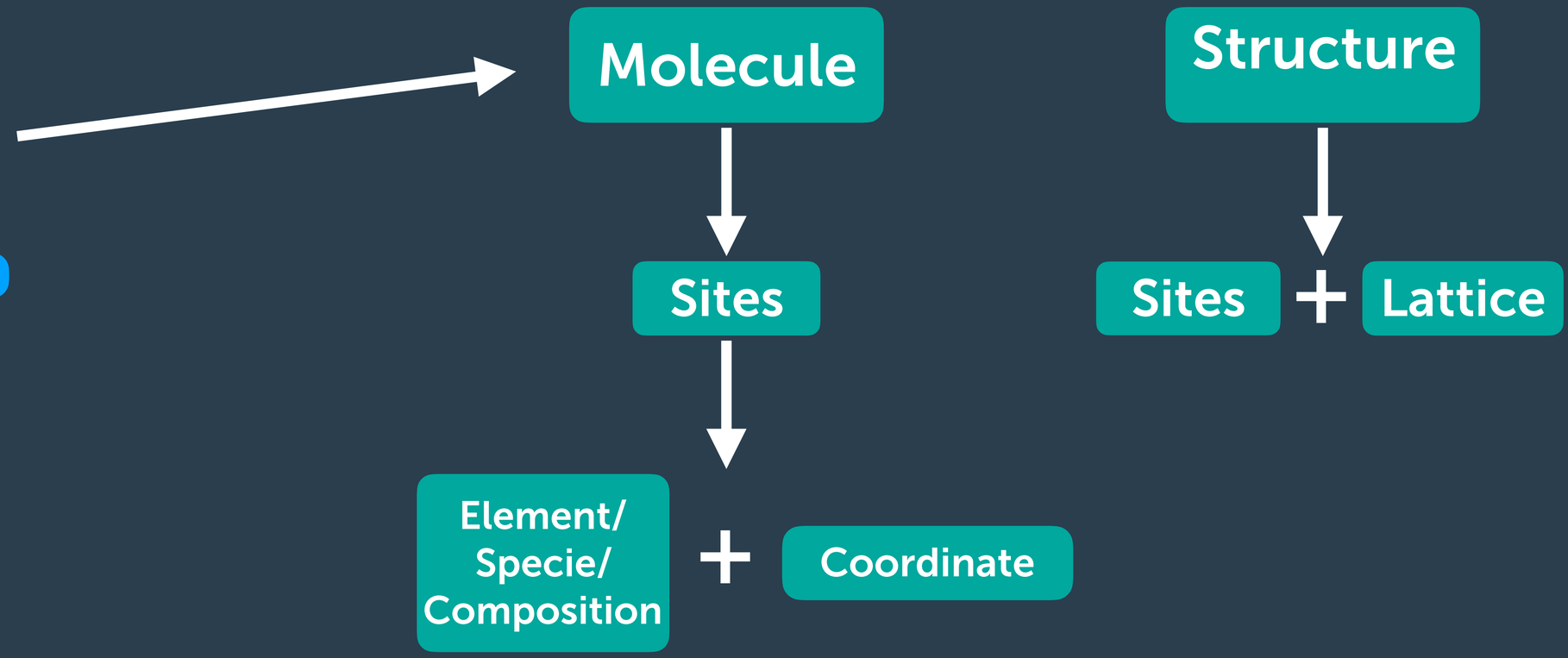
The Materials Project
Workshop 2019

Thursday, 10.45—12pm
Introduction to pymatgen

pymatgen —

The code that powers all scientific analysis in the Materials Project

- alchemy
- analysis
- cli
- apps
- core
- command_line
- electronic_structure
- entries
- ext
- io
- optimization
- phonon
- symmetry
- transformation
- util
- vis



Lunch Break

The Materials Project
Workshop 2019

Thursday, 1.15pm—2.30pm
Advanced pymatgen

Instructors:

Matt

Jianli

In this lesson, you will:

- Learn how to transform crystal structures using pymatgen
- Learn the difference between one-to-one and one-to-many transformations
- Apply to typical use cases

This lesson's notebook can be found at:

`workshop/pymatgen/2 - Advanced Pymatgen - fill in the blanks.ipynb`

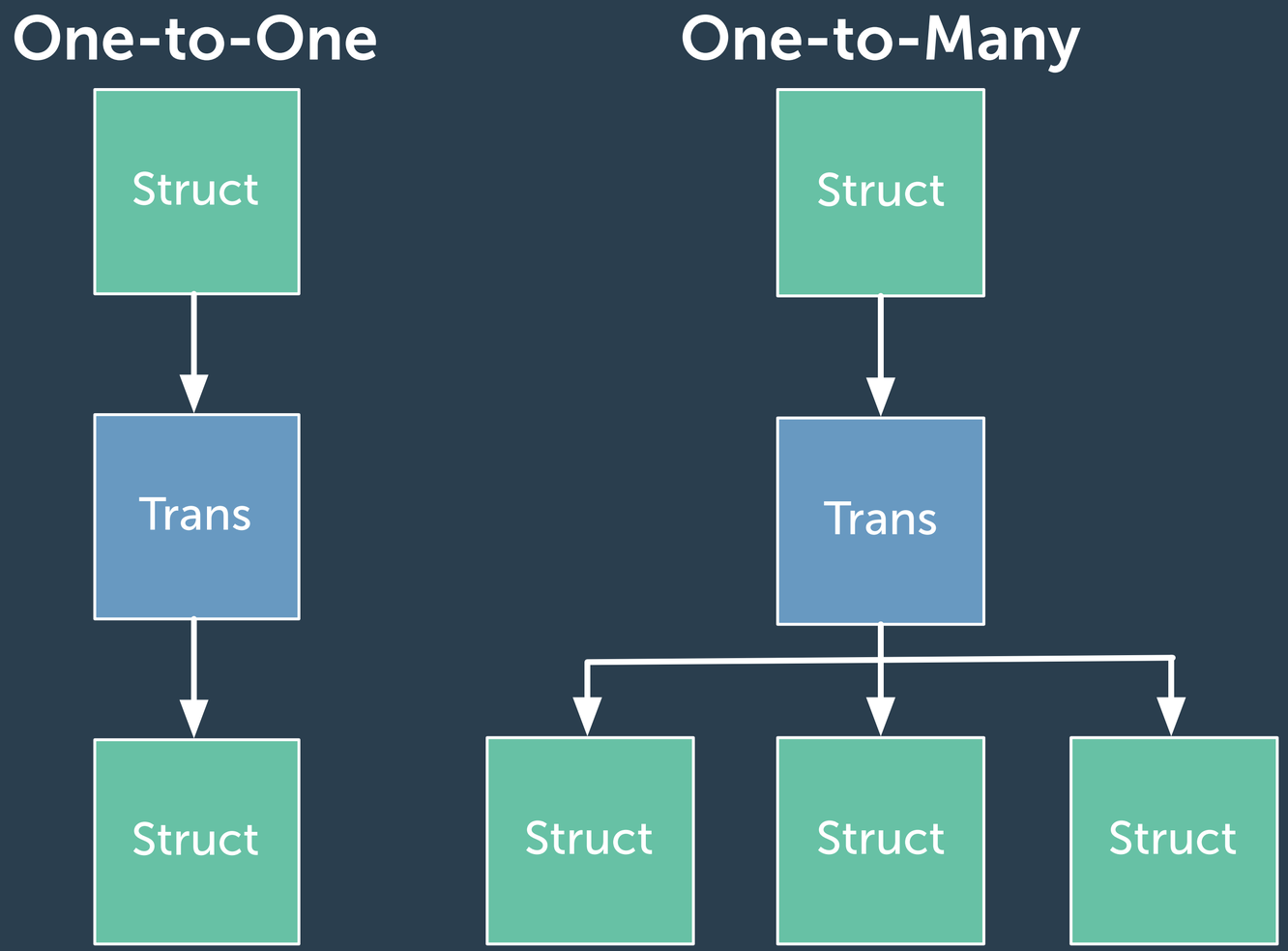
The Materials Project
Workshop 2019

Thursday, 1.15pm—2.30pm
Advanced pymatgen

Instructors:

Matt

Jianli



This lesson's notebook can be found at:

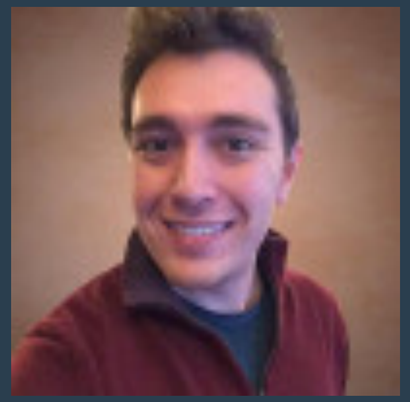
`workshop/pymatgen/2 - Advanced Pymatgen - fill in the blanks.ipynb`

Coffee Break

The Materials Project
Workshop 2019

Thursday, 2.45am—4pm
The Materials Project API

Instructors:



John

Matt

In this lesson, you will:

- Learn more about the Materials Project API (MAPI)
- Learn how to query for MP data using Python
- An example for how to screen the MP database for interesting materials

This lesson's notebook can be found at:

`workshop/MAPI/api_use-empty.ipynb`

The Materials Project
Workshop 2019

Friday, 9.15am—10.30am
Atomate Basics

Instructors:

Eric

Ann

In this lesson, you will:

- Initialize and run standard atomate workflows
- Manage and view fireworks status
- Submit jobs to HPC using fireworks

This lesson's notebook can be found at:

`workshop/atomate/1 - Beginning Workflows_empty.ipynb`

The Materials Project
Workshop 2019

Friday, 9.15am—10.30am
Atomate Basics

Instructors:

Eric

Ann

What is atomate?

- A python package for automating complex materials science computations.
  - VASP, Q-Chem, FEFF, and LAMMPS
  - Band Structure, Elastic tensor, Raman spectra, etc.
- Job tracking and monitoring
- Database storage of calculations including runtime parameters, directories, and outputs.

This lesson's notebook can be found at:

`workshop/atomate/1 - Beginning Workflows_empty.ipynb`

Coffee Break

The Materials Project
Workshop 2019

Friday, 10.45am—12pm
Atomate Advanced

Instructors:

Jimmy

Eric

In this lesson, you will:

- In this lesson, you will learn about:
- Managing a large number of atomate workflows
- Some advanced workflows in atomate
- Manipulate workflows after then have been created
- Analyzing the results of workflows

This lesson's notebook can be found at:

`workshop/lessons/atomate/2 - Workflow management and analysis with atomate.ipynb`

Lunch Break

The Materials Project
Workshop 2019

Friday, 1.15—2.30pm

Contributing Data to Materials Project

Instructors:

Patrick

Donny

In this lesson, you will:

- learn about existing contributed data sets on MP Details Pages
- explore their landing pages on the MPContribs Portal
- use the MPContribs API to retrieve data programmatically

https://mpcontribs.org

This lesson's notebook can be found at:

`workshop/lessons/MPContribs`

Coffee Break

The Materials Project
Workshop 2019

Friday, 2.45—4.00pm
Materials Data Science

Instructors:

Alex G

Alex D

In this lesson, you will:

- Learn how to download and clean datasets using pandas
- Convert pymatgen objects into machine learnable features
- Train and evaluate a machine learning model to predict elastic constants

This lesson's notebook can be found at:

`workshop/lessons/matminer`