

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

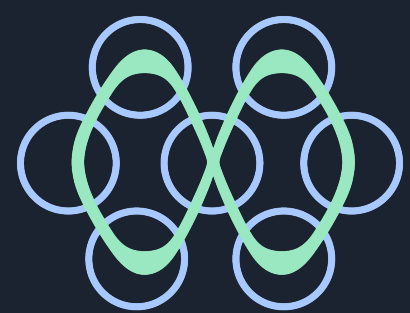
3. Case studies on how to use pymatgen to transform crystal structures
4. Accessing MP data with code using pymatgen

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



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Feedback and Help



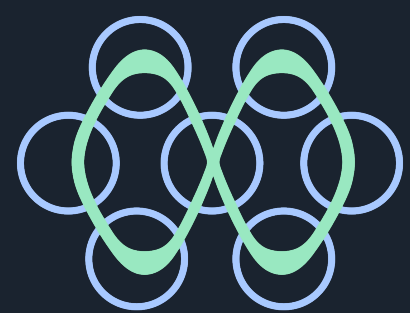
Ask us questions on Slack
mpworkshop.slack.com



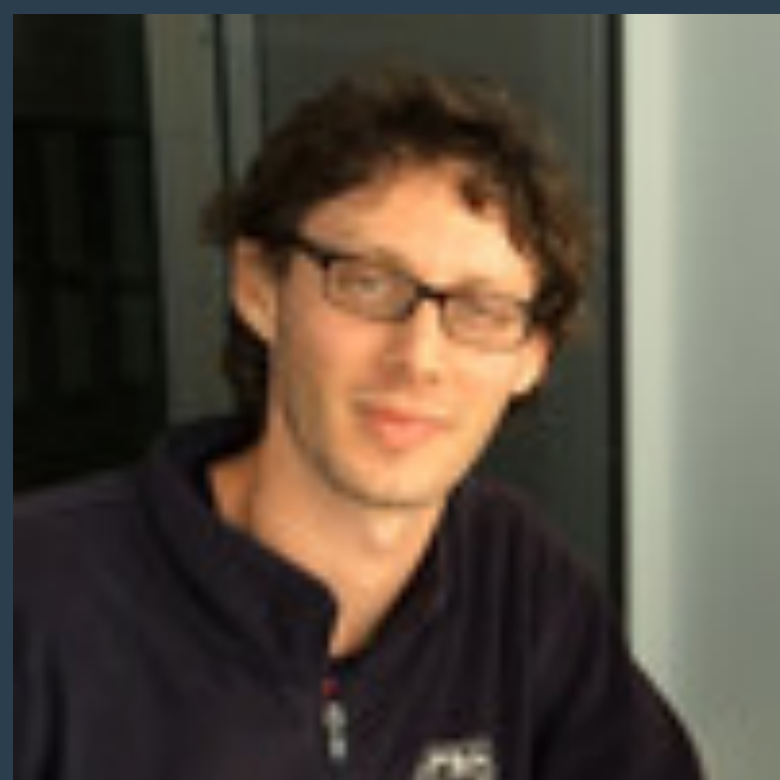
Answer exercises during lessons + give
feedback: pollev.com/mpworkshop



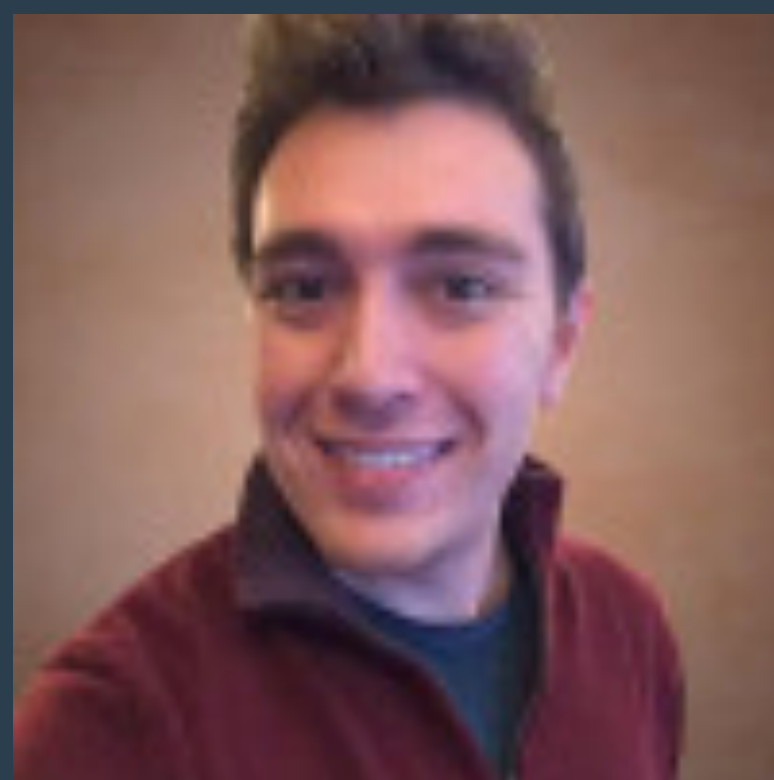
Put up a sticky note on your laptop!
Green is good, red means help



Instructors:



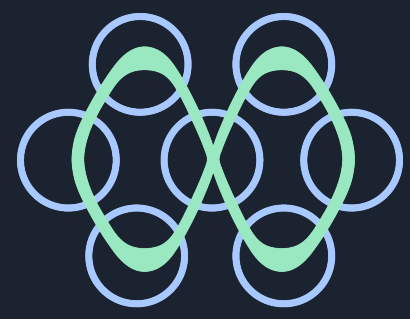
Donny



John

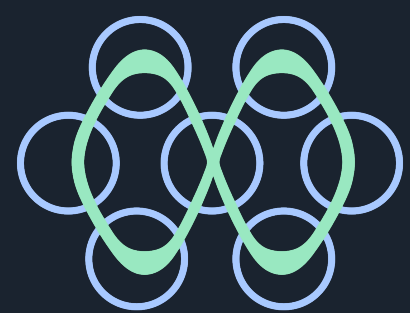
In this lesson, you will:

- 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



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Coffee Break



Instructors:



Sam



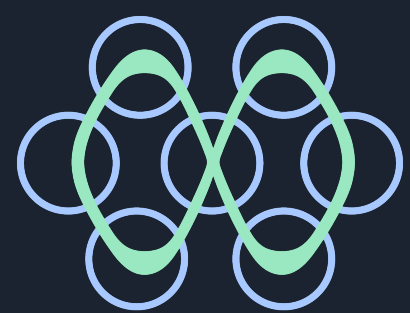
Alex

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`



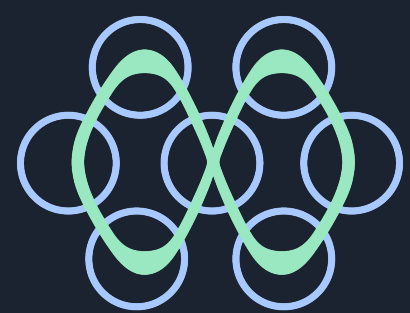
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Thursday, 9—10.30am
Introduction to pymatgen

pymatgen

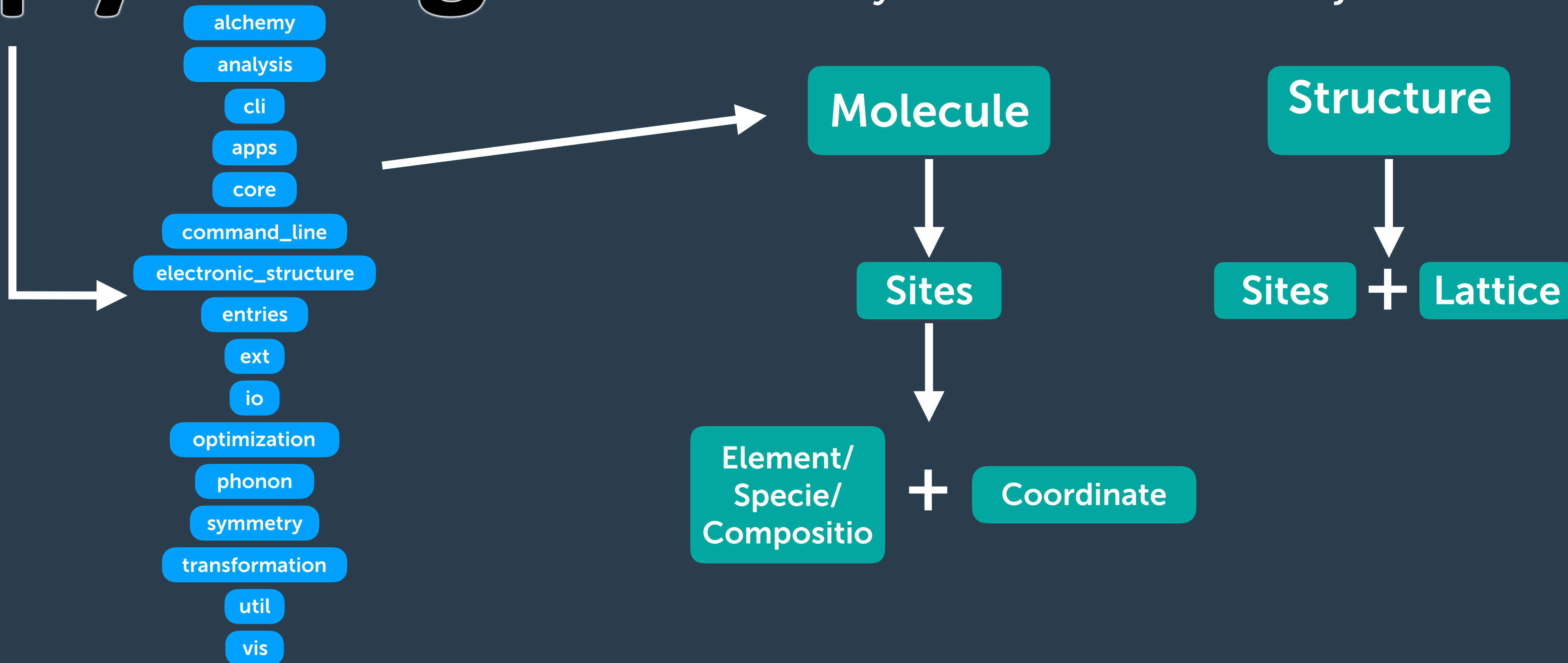
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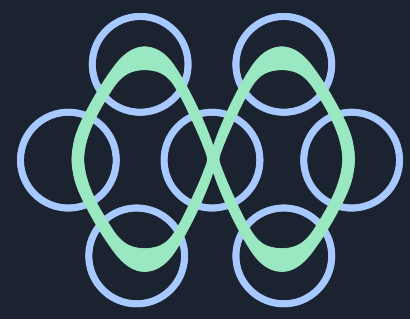
The code that powers all scientific
analysis in the Materials Project



pymatgen

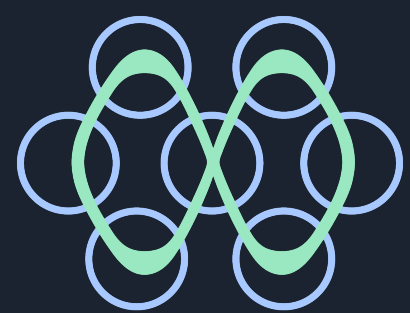
The code that powers all scientific
analysis in the Materials Project





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Lunch Break



Instructors:



Matt



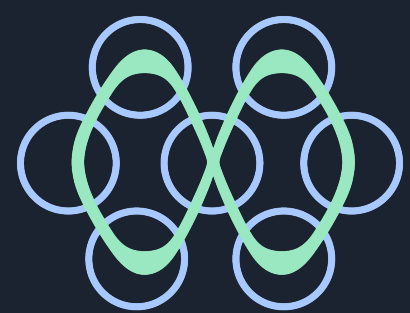
Jianli

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`



Instructors:

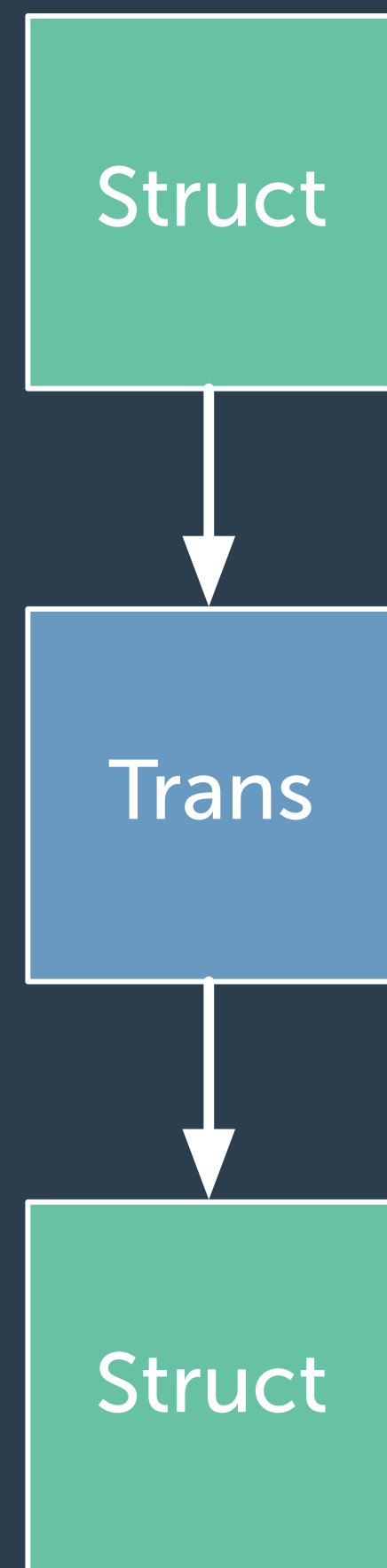


Matt

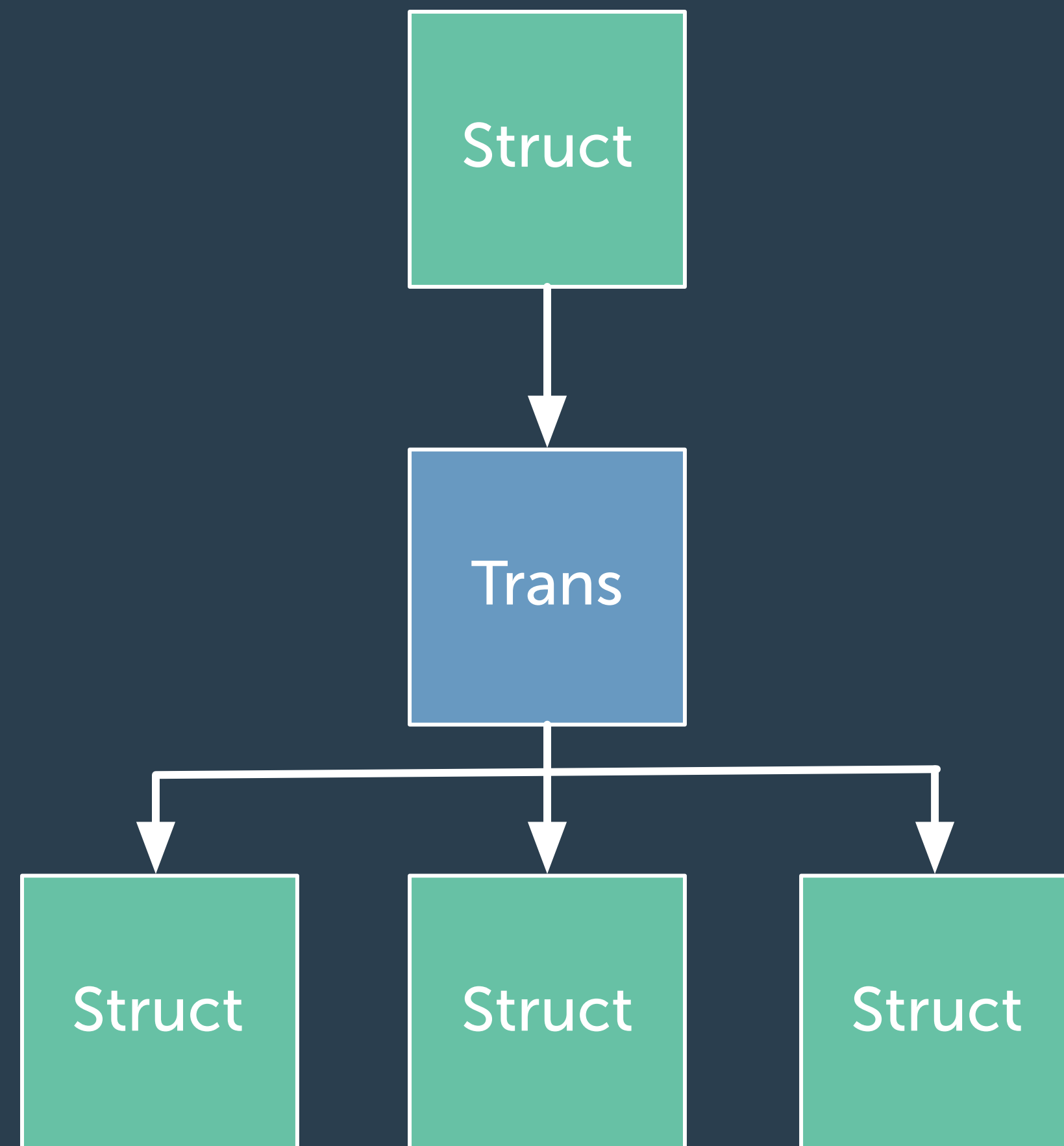


Jianli

One-to-One

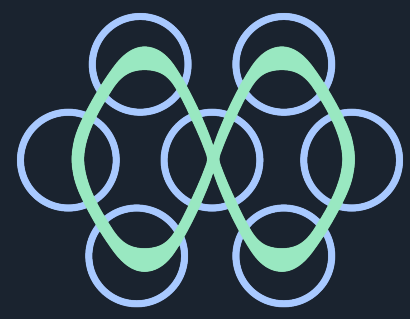


One-to-Many



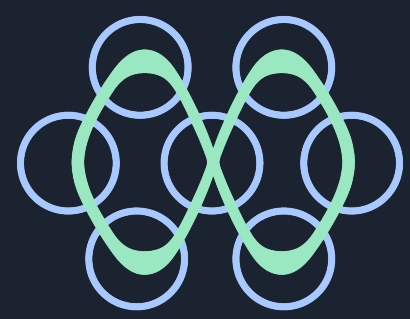
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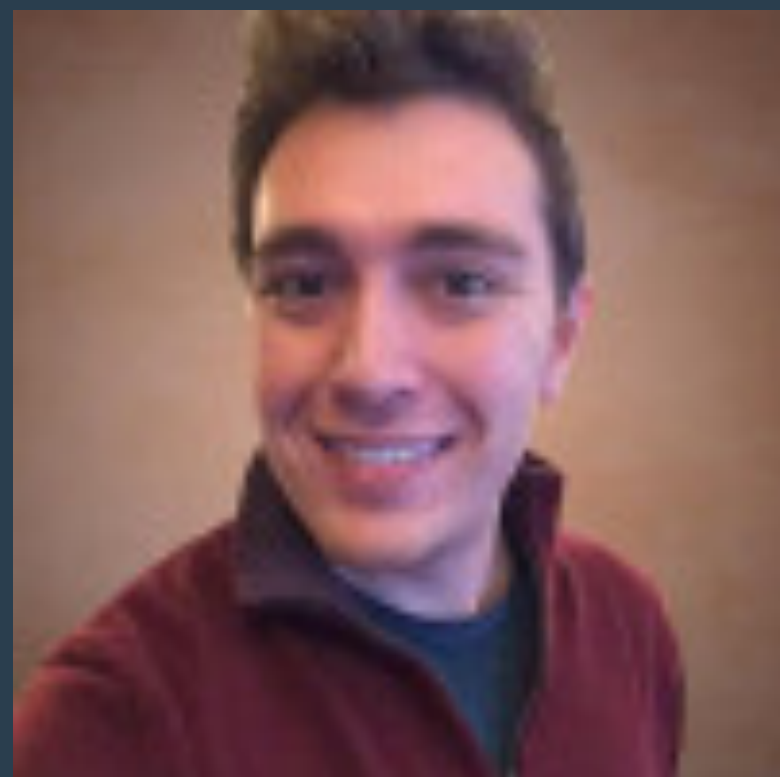


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Coffee Break



Instructors:



John



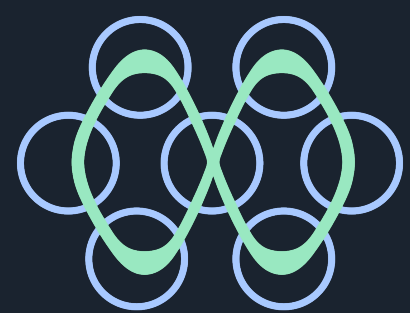
Matt

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`



Instructors:



Eric



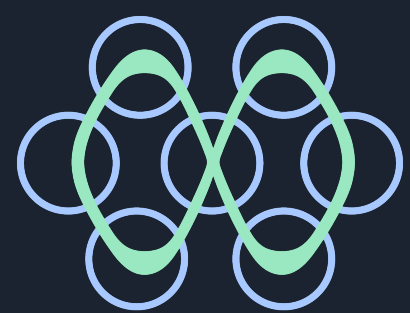
Ann

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`



Instructors:



Eric



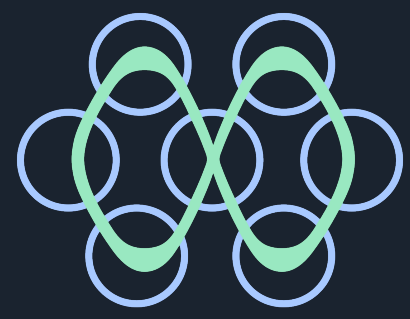
Ann

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.

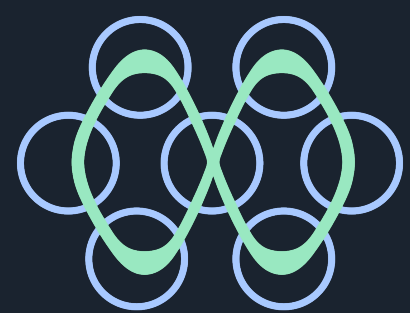
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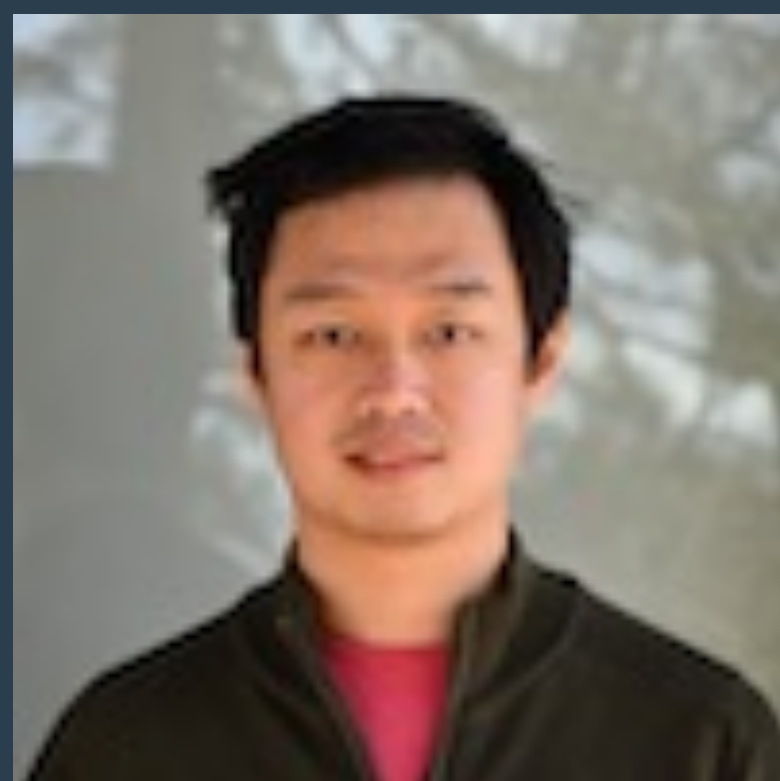


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Coffee Break



Instructors:



Jimmy



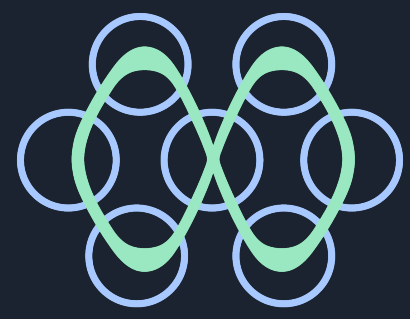
Eric

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

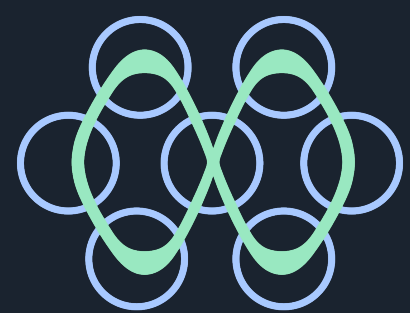
This lesson's notebook can be found at:

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



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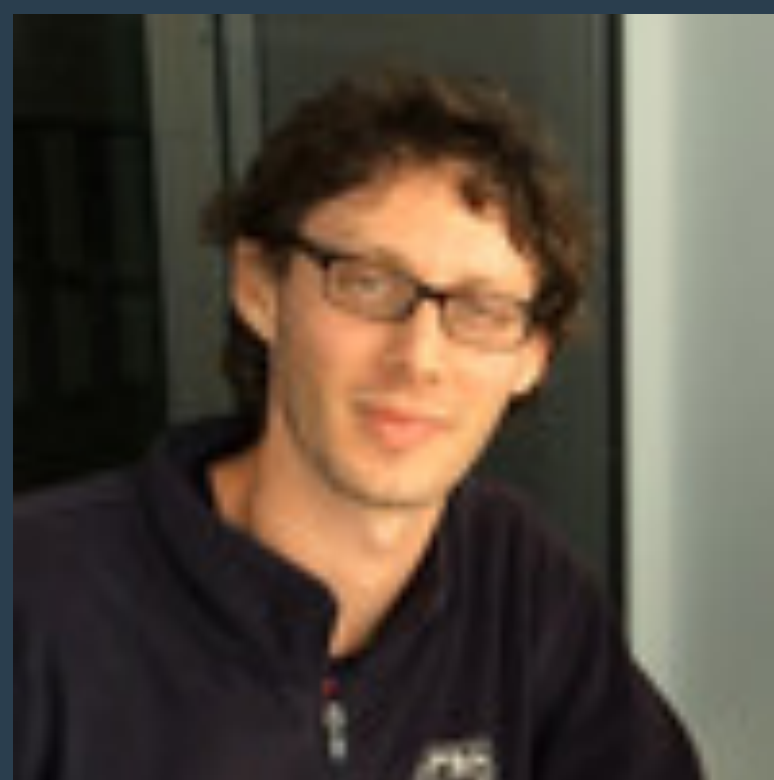
Lunch Break



Instructors:



Patrick



Donny

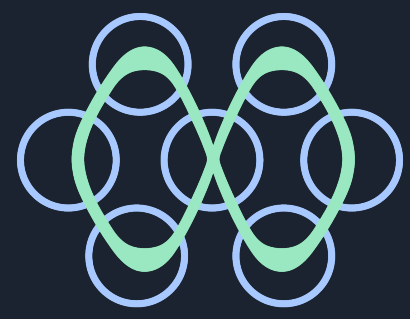
In this lesson, you will:

- 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>

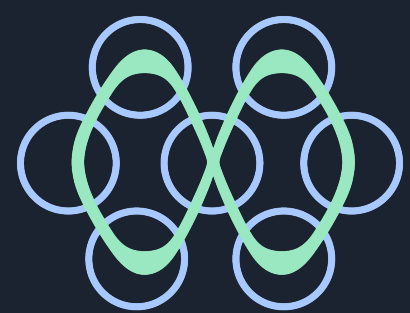
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`workshop/lessons/atomate/MPContribs`



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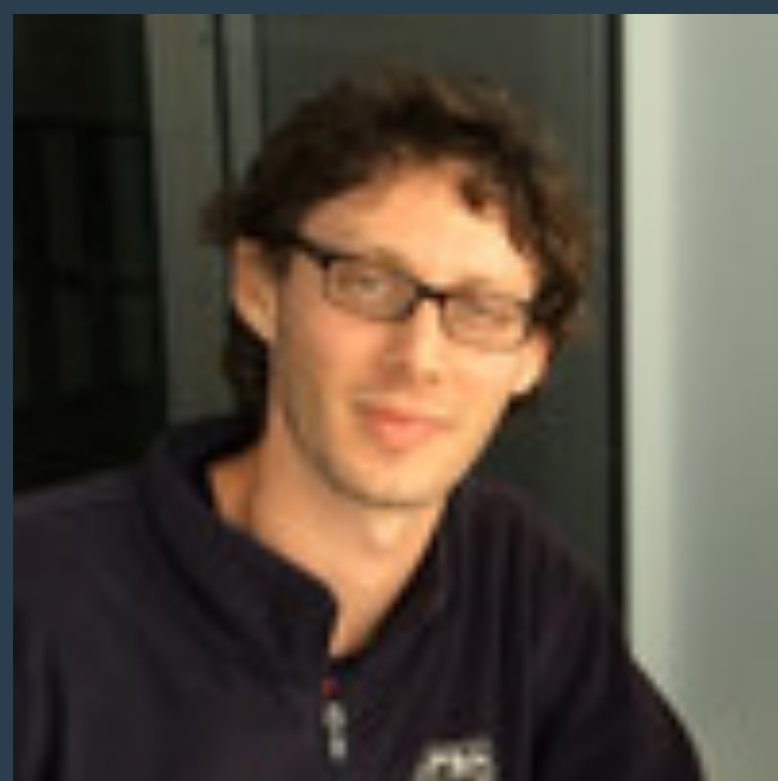
Coffee Break



Instructors:



Patrick



Donny

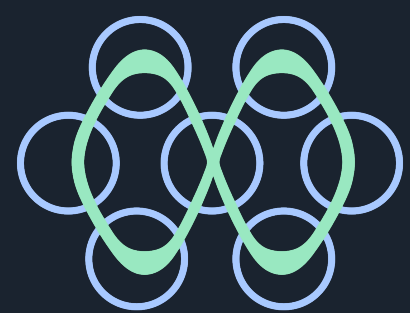
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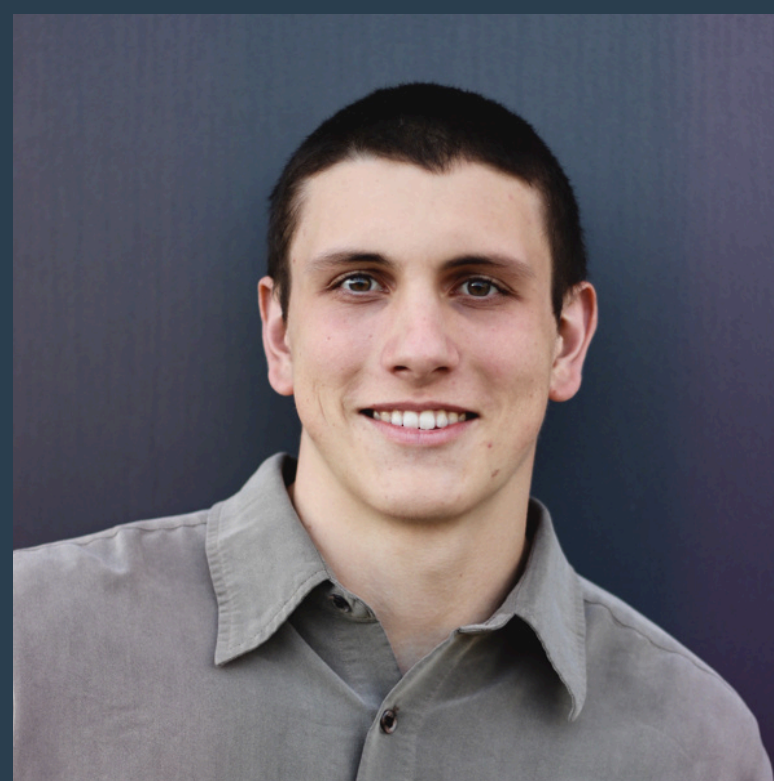
`workshop/lessons/atomate/MPContribs`



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`