The Materials Project and High-Throughput DFT

MSE 215 Guest Lecture: Nov 19, 2019

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BERKELEY LAB

Schedule (Original)

Tuesday:

Introduction to the Materials Project
MP Website Walkthrough
The Story of High Throughput DFT

Thursday:

Materials Project Lab

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Schedule (Revised)

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If class is canceled on Thursday we will share recorded lectures that cover this content.

Quick Setup

1. Go to:

github.com/mse215/mplectures

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4. Get repo with

```
>> git clone <paste_url>
```

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5. Create Conda Env

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>> conda create -n mse215 python=3
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6. Activate Env

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(Error? try `source activate mse215`)

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7. Enter mplectures directory

```
>> cd mplectures
```

Quick Setup

8. Install dependencies

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>> pip install -r requirements.txt
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9. Wait for installation to finish while I talk for a bit...

Pip install pymatgen

What is the Materials Project?

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Data + Software + Dissemination

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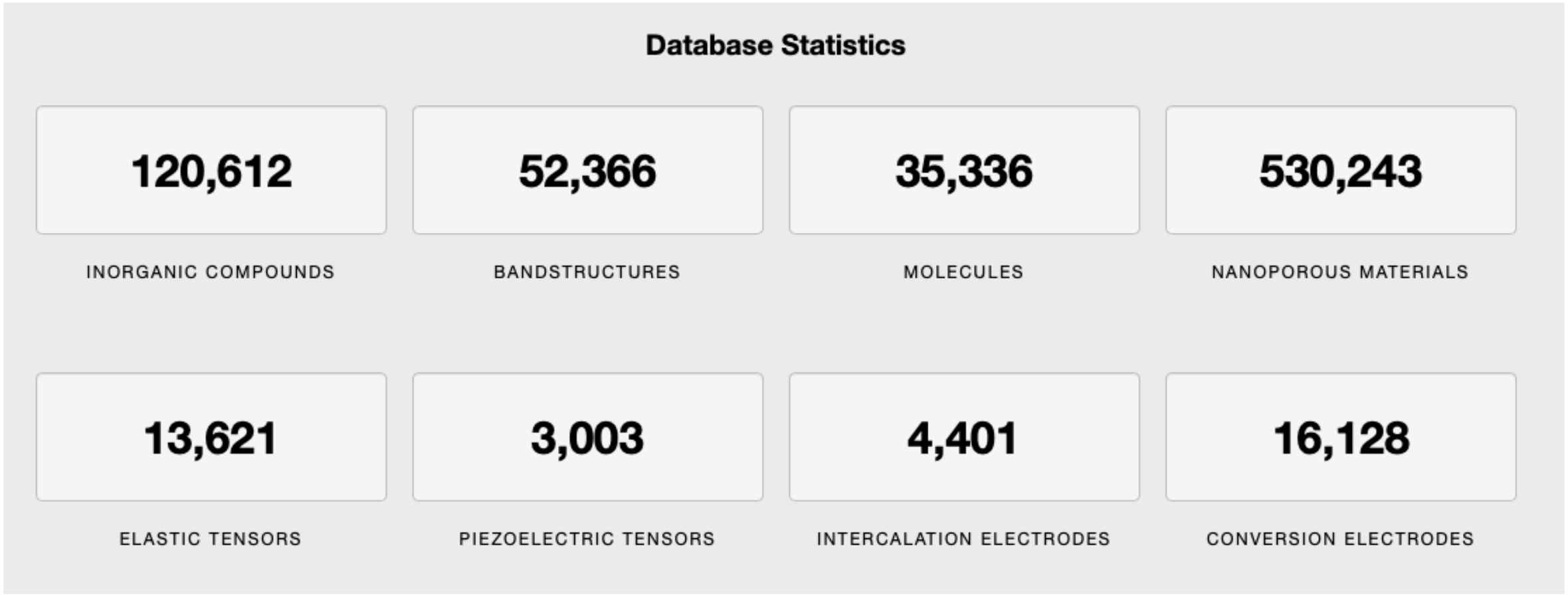
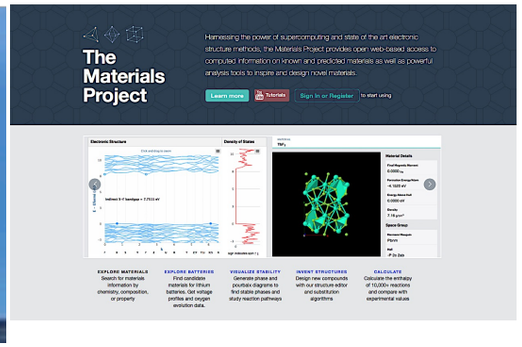
More on Thursday!

Materials Data



materialsproject.org

Website it just the tip of the iceberg



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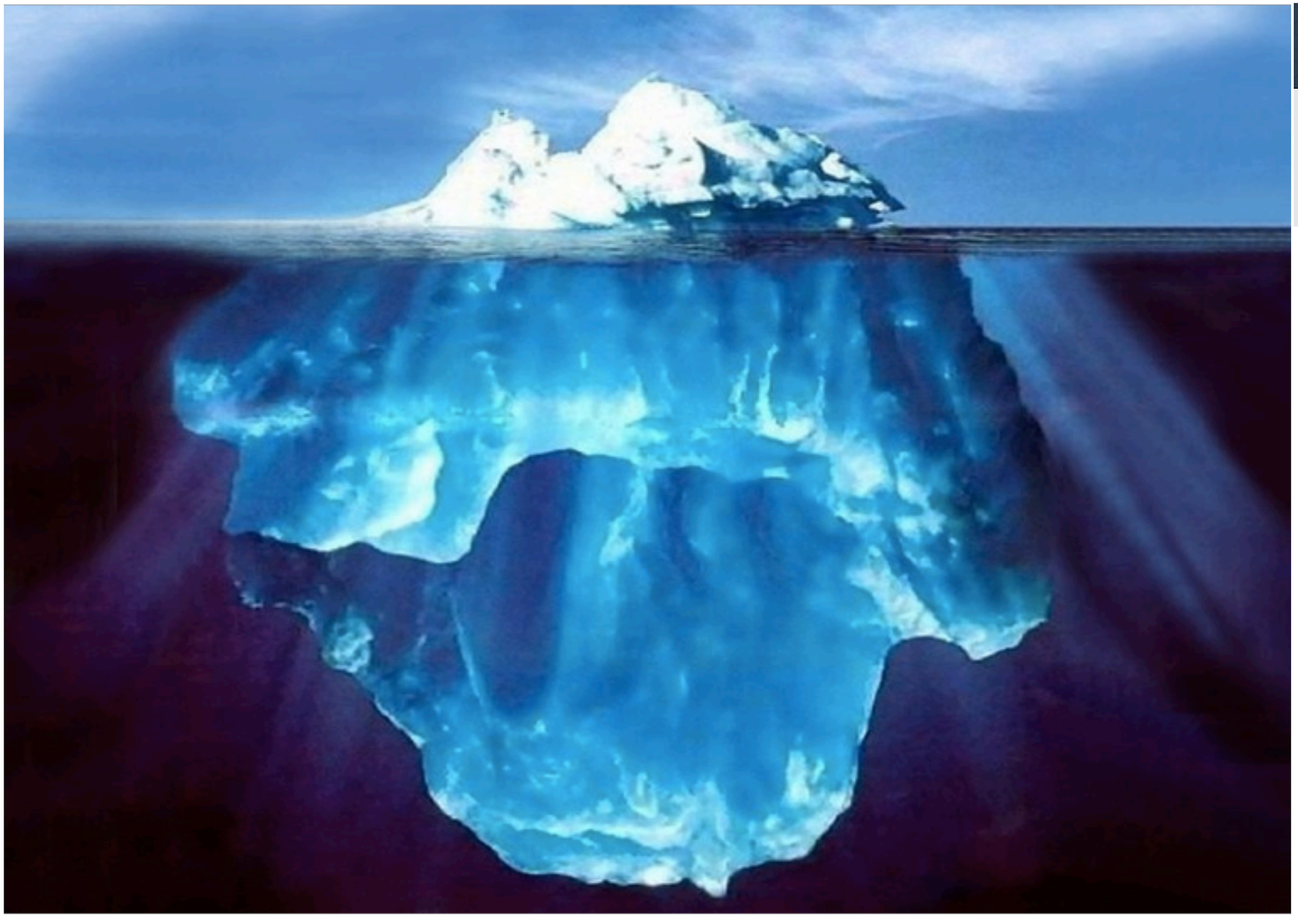
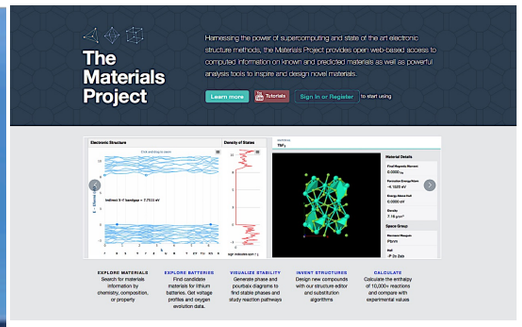




pymatgen

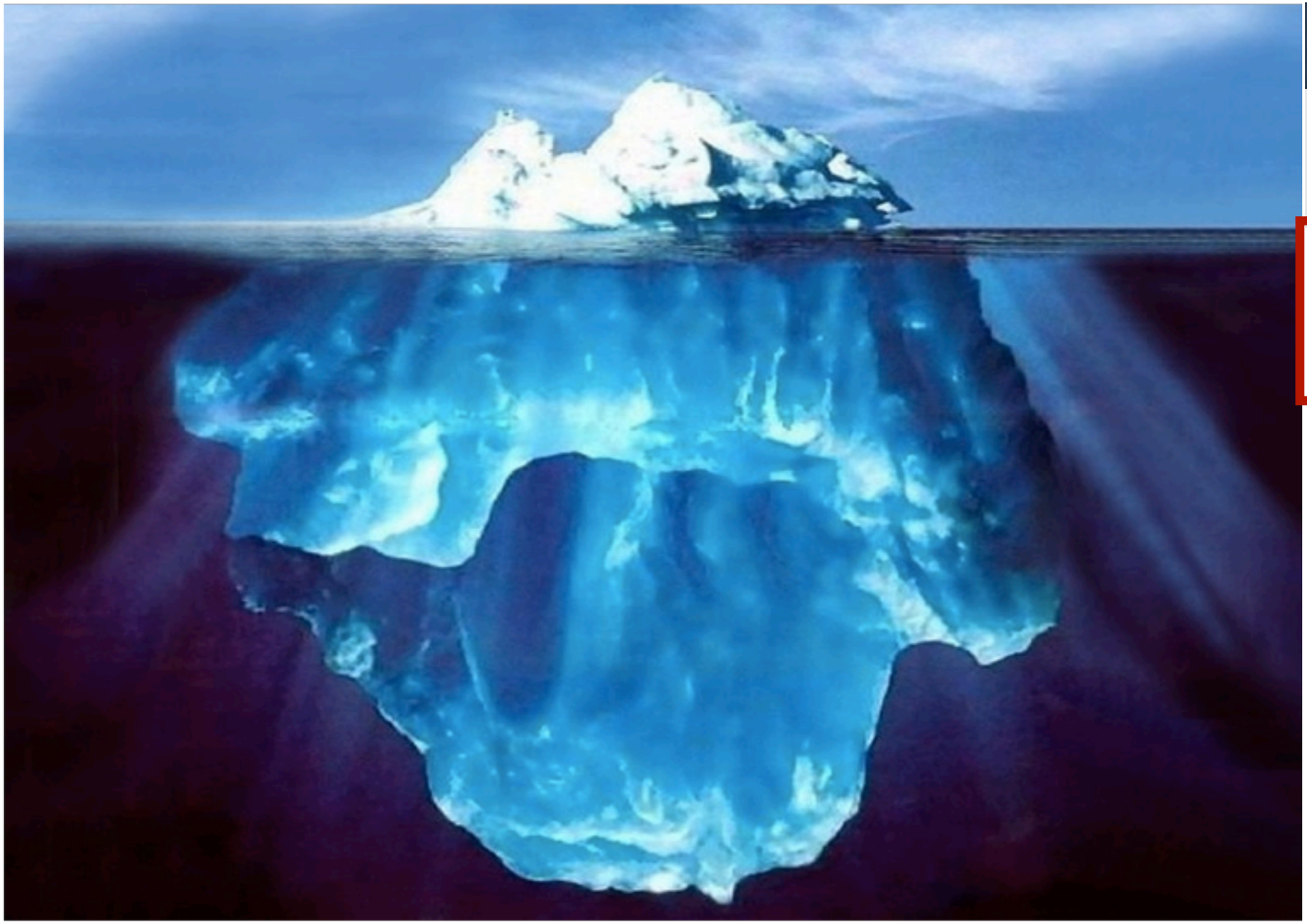
Custodian

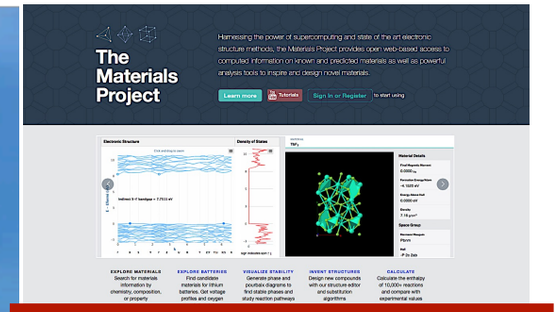
FireWorks

atomate

Emmet

Website it just the tip of the iceberg





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Pymatgen Lab

Time for some
hands on (keyboard) learning!

```
>> jupyter notebook
```

Thank You!

@jmdagdelen

Questions?