

The 2016 Materials Project Workshop

*Kristin Persson
UC Berkeley*

*With immense thanks to the team, without
which nothing would have happened and we
wouldn't be here today*

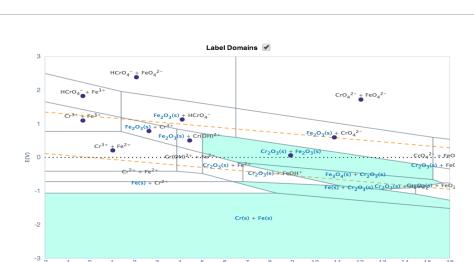
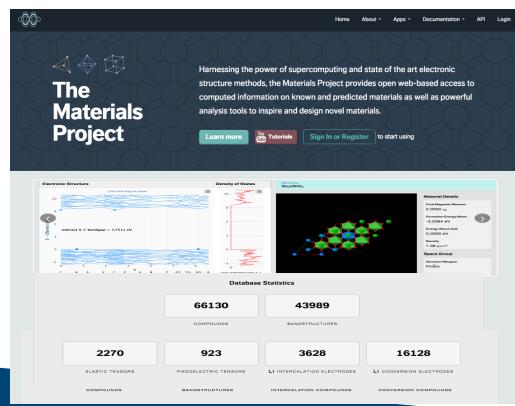


First-Principles Modeling: 1996 - 2016

1996: One year on tungsten

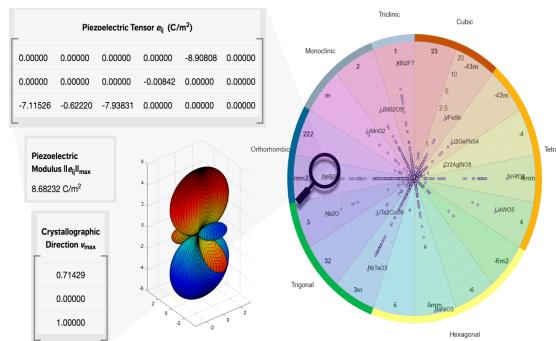
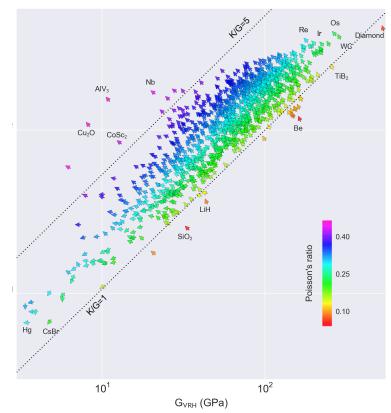


2016: 66,000+ materials on the Materials Project + millions of materials properties



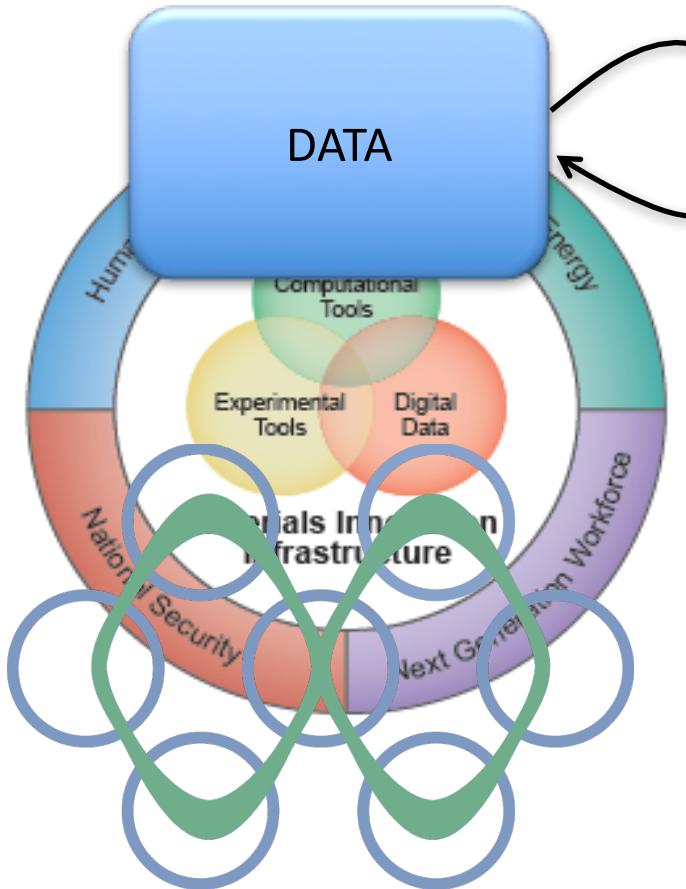
Pourbaix Diagrams on the Materials Project

Today, we are excited to announce the release of the [Pourbaix diagram app](#). Pourbaix diagrams are solid-aqueous phase diagrams as a function of pH, standard hydrogen potential and composition that can be used to



Piezoelectricity Data on the Materials Project

The MGI and the Materials Project



June 2011 “fund **computational tools, software, new methods ... to make the process of discovery and development of advanced materials faster, less expensive, and more predictable**
Bring unprecedented high quality materials data from first-principles,

Integrate it with state-of-the-art information technology and codes to enable rapid **dissemination**, searching, datamining and enhanced learning

Demonstrate capabilities on **design** of novel functional electronic materials

Materials Project web site

The Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

[Learn more](#) [Sign In or Register](#) to start using

Electronic Structure
Click and drag to zoom
Indirect X- Γ bandgap = 7.7511 eV
E - E_{Fermi} (eV)

Density of States

MATERIAL
Ba2UNiO6

Material Details

- Final Magnetic Moment
2.0000 μ_B
- Formation Energy/Atom
-3.0384 eV
- Energy Above Hull
0.0000 eV
- Density
7.38 g/cm³
- Space Group
Hermann Mauguin
Fm $\bar{3}$ m
Hall

EXPLORE MATERIALS
Search for materials information by chemistry, composition, or property

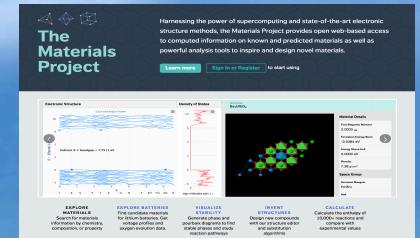
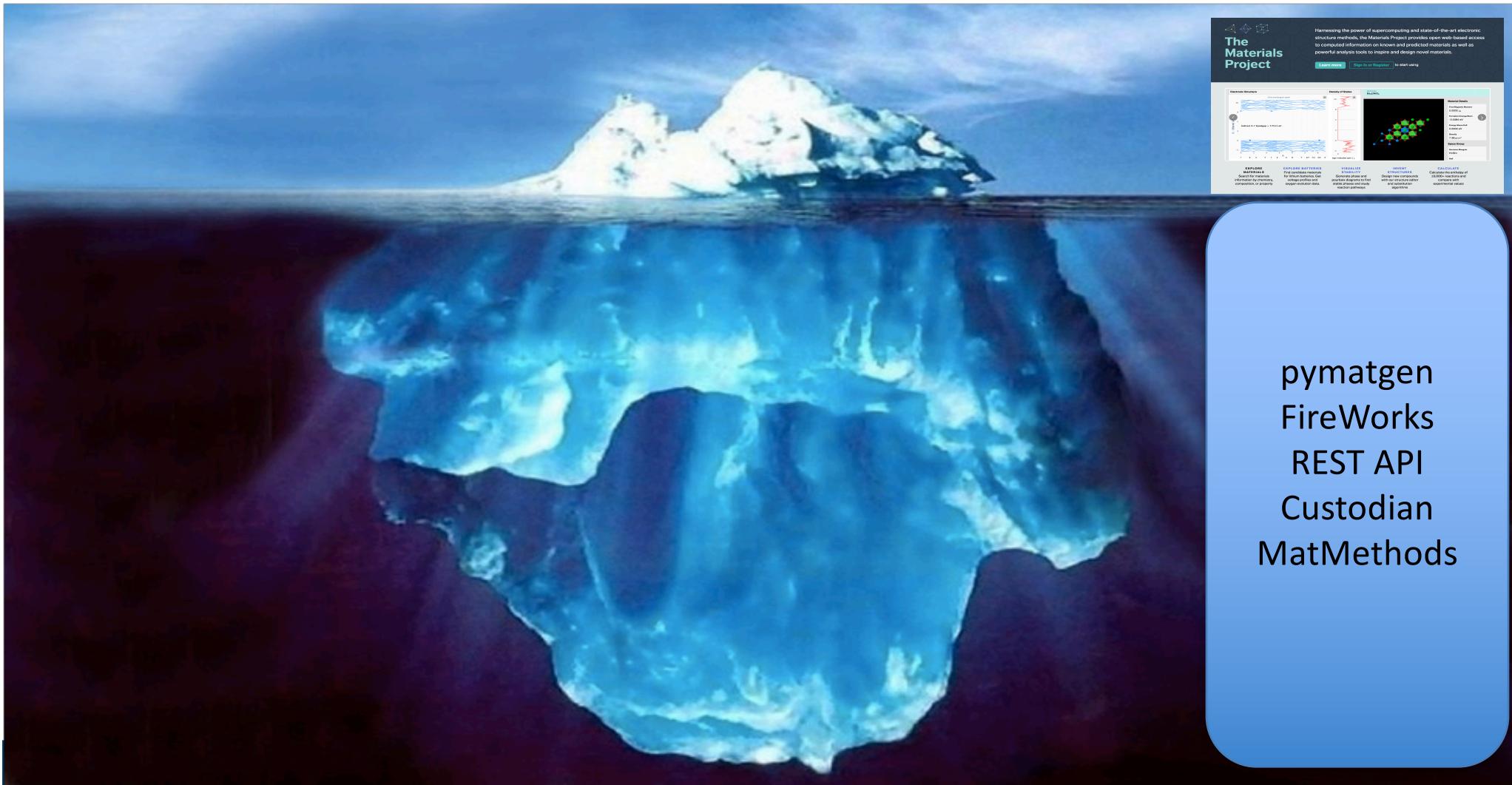
EXPLORE BATTERIES
Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

VISUALIZE STABILITY
Generate phase and pourbaix diagrams to find stable phases and study reaction pathways

INVENT STRUCTURES
Design new compounds with our structure editor and substitution algorithms

CALCULATE
Calculate the enthalpy of 10,000+ reactions and compare with experimental values

The web site is the tip of the iceberg...



pymatgen
FireWorks
REST API
Custodian
MatMethods

ICSD

Other experimental databases

User submissions

Input processing & transformations

StructureNotationalLanguage (SNL)



Analysis

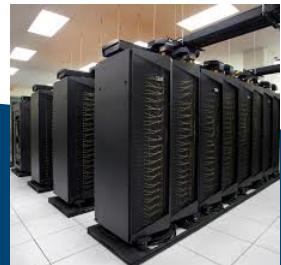
Web apps

Materials API

Workflow Manager

Post-processing and
error-checking

Supercomputing Resources



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ICSD

Other experimental databases

User submissions

Input processing & transformations

pymatgen

- Robust materials analysis



Custodian

- Self-healing error recovery



Fireworks

- Smart workflow management



StructureNotationalLanguage (SNL)



Analysis

Workflow Manager

Post-processing and error-checking

Web apps

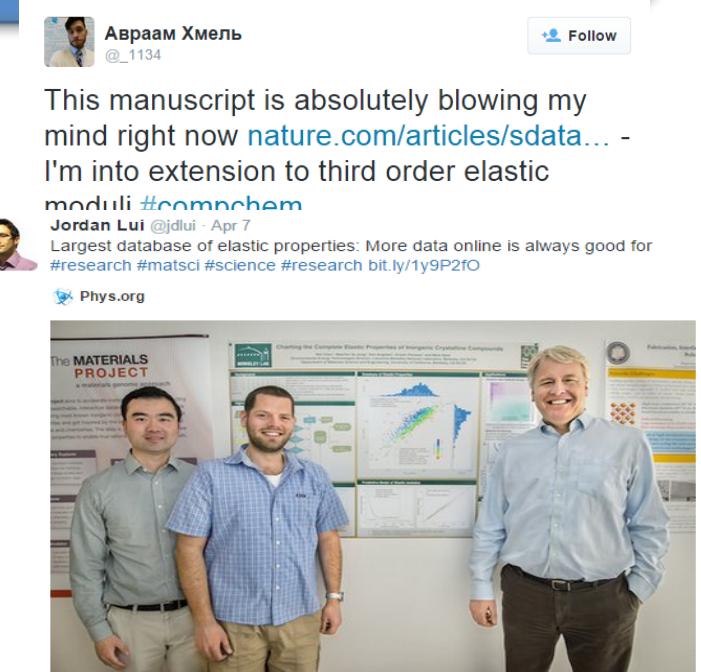
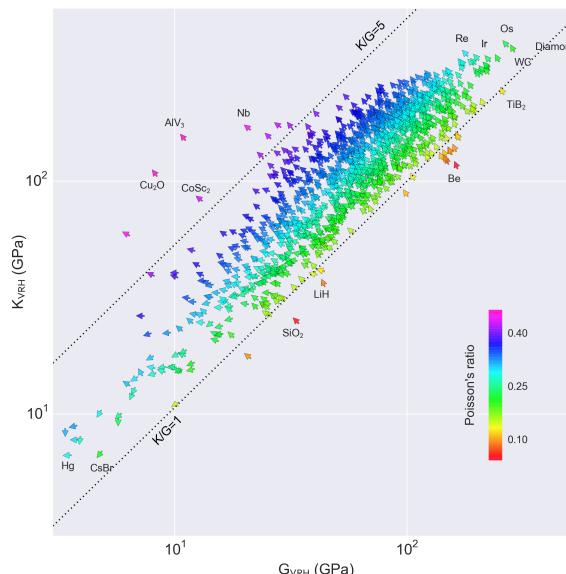
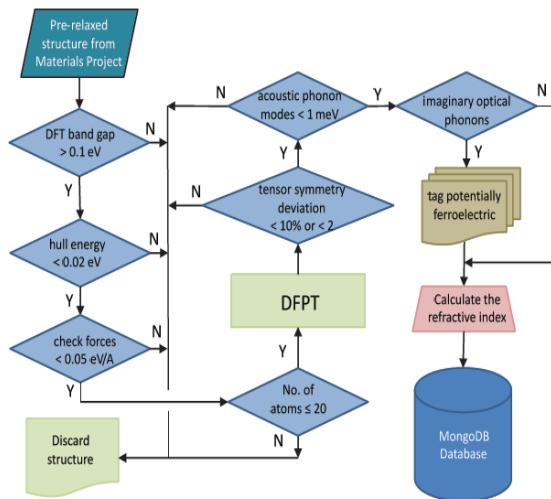
Materials API

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Supercomputing Resources

All HT Properties Benchmarked and Automated



MP Apps

Electronic structure
Phase diagrams
Battery properties
Pourbaix Diagrams
Organic molecules
Design Center
...

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The screenshot shows the Materials Project's 'Explore Materials' interface. At the top, there is a search bar with the placeholder 'Search for materials information by chemistry, composition, or property'. Below the search bar is a navigation bar with icons for user profile, search, email, tools, and help. A green box highlights the search bar and the sidebar filters.

The main area features a periodic table where elements can be selected. A search bar with the query 'Fe Li S' is positioned above a results table. The results table displays 10 entries of Fe-Li-S compounds, including their Materials ID, formula, spacegroup, formation energy (eV), energy above hull (eV), band gap (eV), number of sites, density (gm/cc), and volume. The table includes buttons for 'records per page' (set to 10), 'Batch Structures', 'Edit Structures', and 'Show / hide columns'.

The right side of the interface is a sidebar with various filters:

- # of elements: e.g., 4 or >2 & <6
- excluded elements: Cl Br
- Submit
- Material Tags: imgreite
- Band Gap (eV): slider from 0 to 10, currently at ~5
- Energy Above Hull: slider from 0 to 6, currently at ~3
- Formation Energy: slider from -4 to 4, currently at ~0
- # unit cell sites: slider from 1 to 296, currently at ~150
- Density: slider from 0 to 24.6, currently at ~12
- Volume: slider from 7 to 7697, currently at ~3000
- Crystal Systems: Any
- Spacegroup Number: Any
- Spacegroup Symbol: Any
- Has bandstructure: checked

MP Going Interactive: MPComplete and MPContribs

