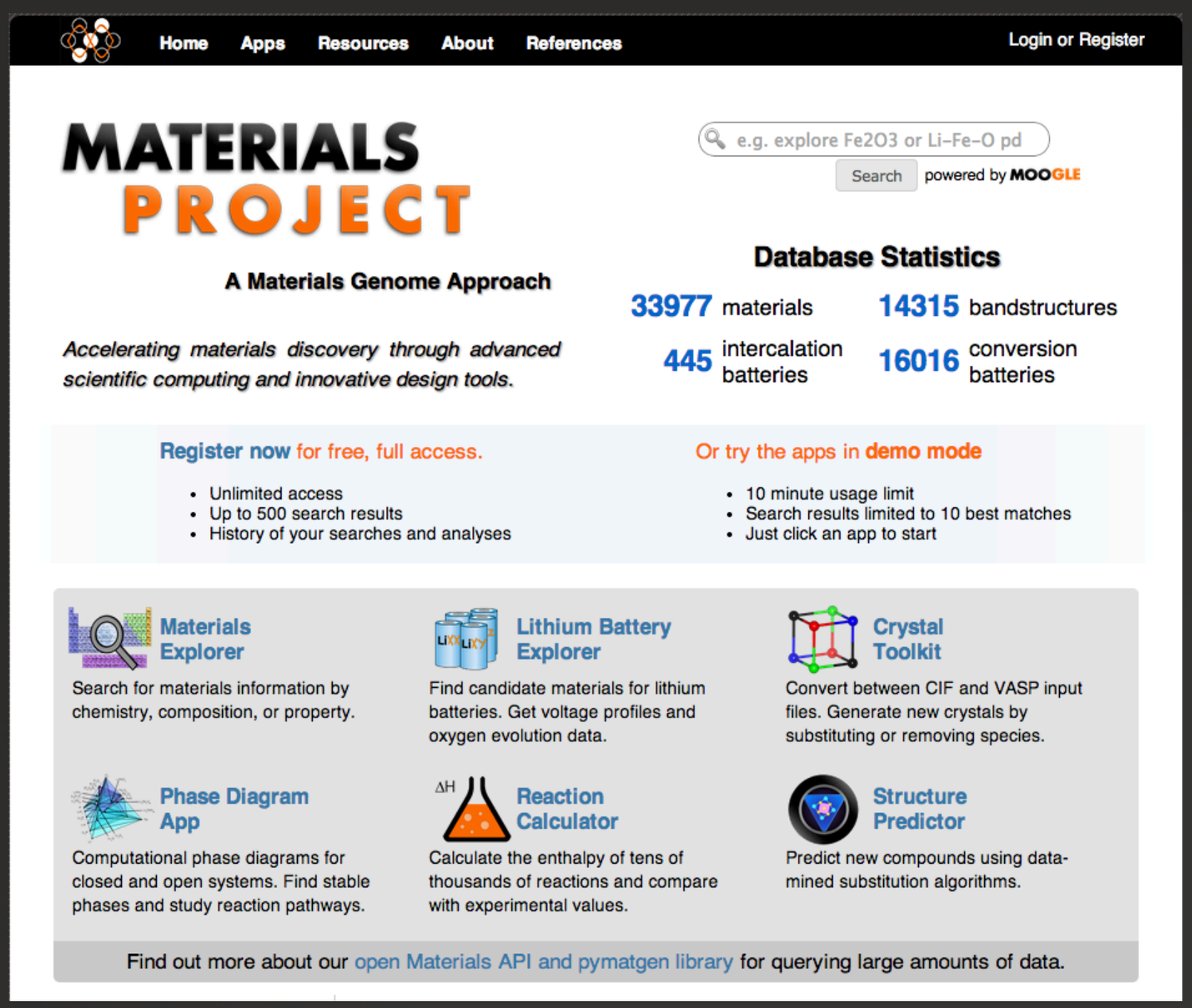
Bringing Better Materials to Market in Half the Time



Researchers are using calculations performed at NERSC to replace trial and error and educated guesses with a systematic approach to designing materials for better batteries, solar cells, electric vehicles, hydrogen storage, catalyst design, and fuel cells.

Scientists scan the Materials Project database of pre-computed material properties to find one that is best for their application. The most promising candidates are then synthesized and studied, greatly accelerating the pace of materials discovery. The goal of the Materials Project is to cut in half the 18 years it takes to move materials from lab to market.

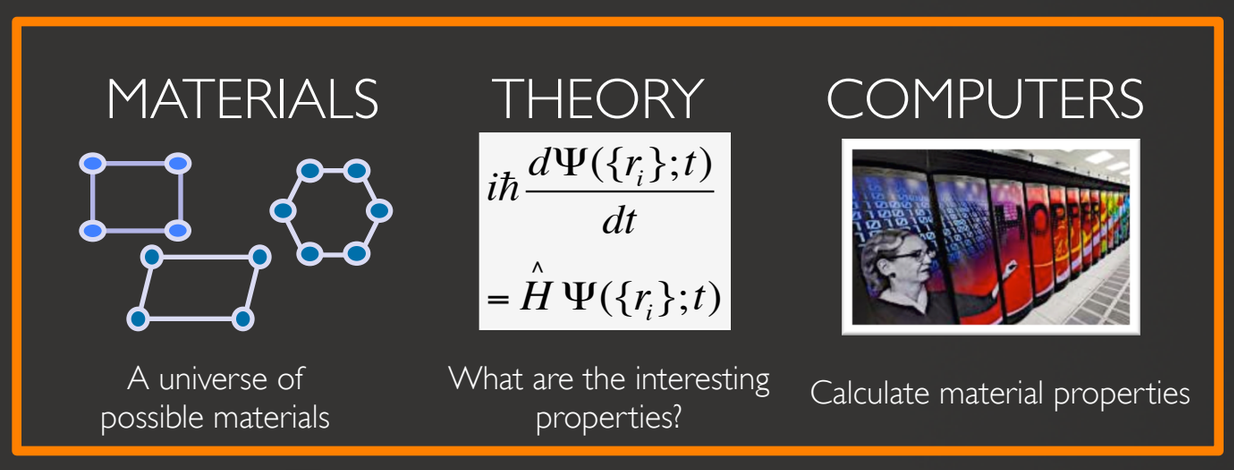
The database of pre-computed properties comprises some 35,000 materials, all accessible through a web-based NERSC Science Gateway: The Materials Project (https://materialsproject.org).

The Materials Project brings together the four pillars of science: experiment, theory, computation, and data-driven discovery.

From the large space of possible materials, theory tells how to determine the interesting properties based on the material's chemistry and crystal structure, computers do the actual calculations, and experimentalists synthesize materials and measure their properties.

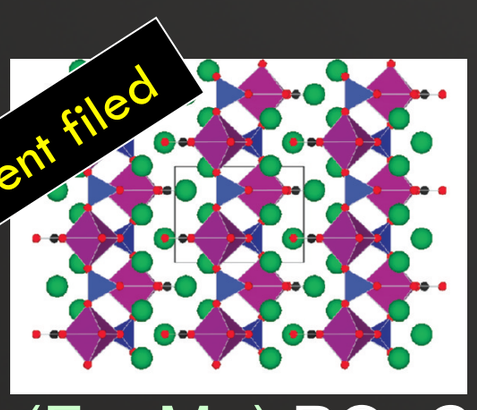
By screening through the 35,000 pre-computed compounds (data-driven discovery) during the early phase of the Material Project scientists identified several materials for better Li-ion batteries that have been synthesized and are being patented (see below).

Expanding into the vast space of more complex properties will have extreme computing needs.



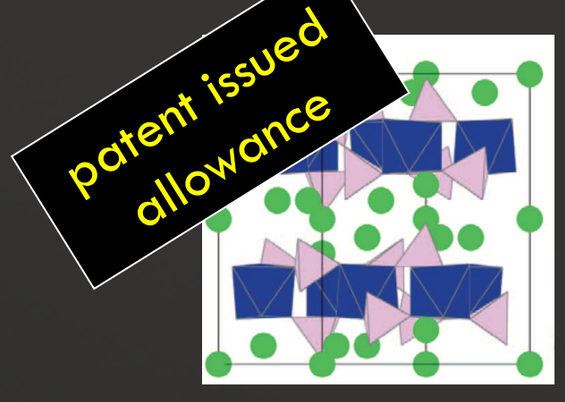
Search DATA: Are the calculated properties interesting?

Do not synthesize!
Put on back burner
Investigate in the lab



$Li_3 (Fe, Mn) PO_4 CO_3$

Hautier, Jain, Moore, Chen, Moore, Ong, Ceder
Journal of Materials Chemistry (2011)
Chen, Hautier, Jain, Moore, Kang, Doe et al.
Chemistry of Materials (2012)



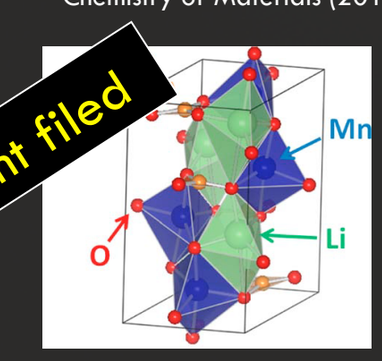
$Li_9 V_3 (P_2O_7)_3 (PO_4)_2$

Jain, Hautier, Moore, Kang, Lee, Chen, Twu, Ceder
Journal of the Electrochemical Society (2011)

New Cathodes Found for Li-ion Batteries

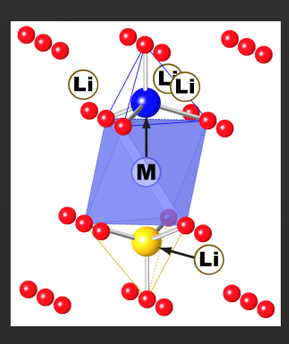
Rechargeable Lithium-Ion batteries are commonly used in consumer electronics. With excellent energy density and the ability to reversible cycle thousands of times, Li-Ion batteries have a great potential for use in the automotive and aerospace industries.

In order to achieve their potential however, new compounds with improved characteristics will be required to, for example, power a car for 300 miles. Here, the Material Project is already making a big impact, having identified many potential candidate materials, some of which are shown at left.



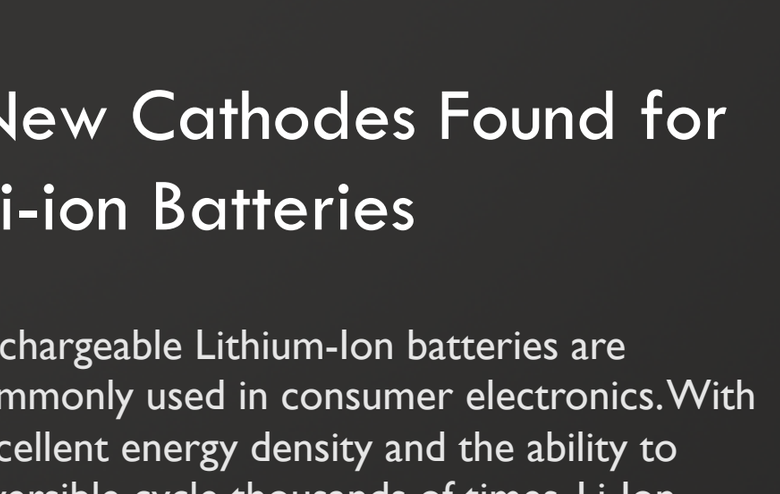
$Li\ Mn\ BO_3$

Kim, Moore, Kang, Hautier, Jain, Ceder
Journal of the Electrochemical Society (2011)



$Li\ (V, Cr)\ O_2$

Ma, Hautier, Jain, Ceder
Journal of the Electrochemical Society (submitted)



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