New materials discovery using simulation, machine learning, and automated laboratories

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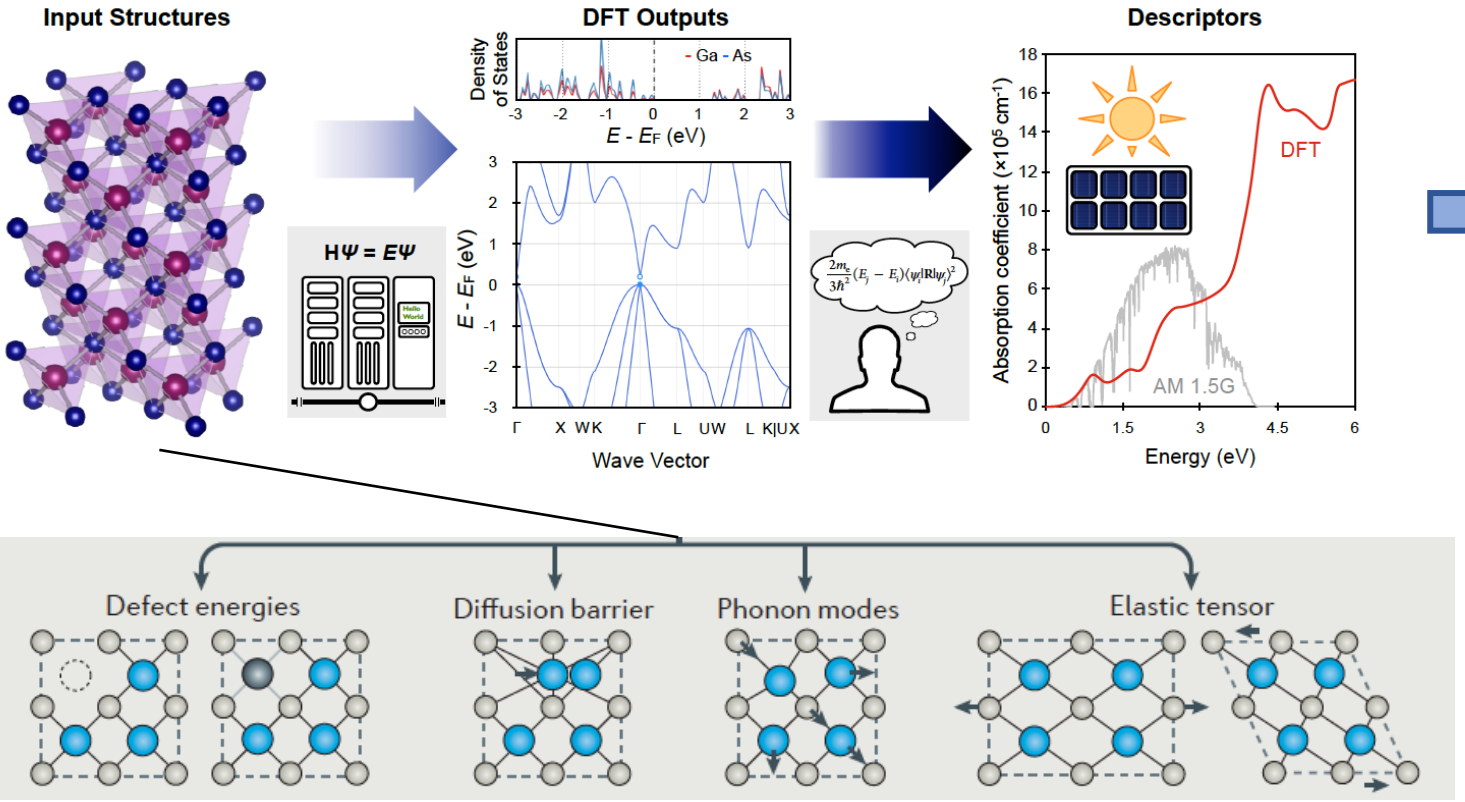
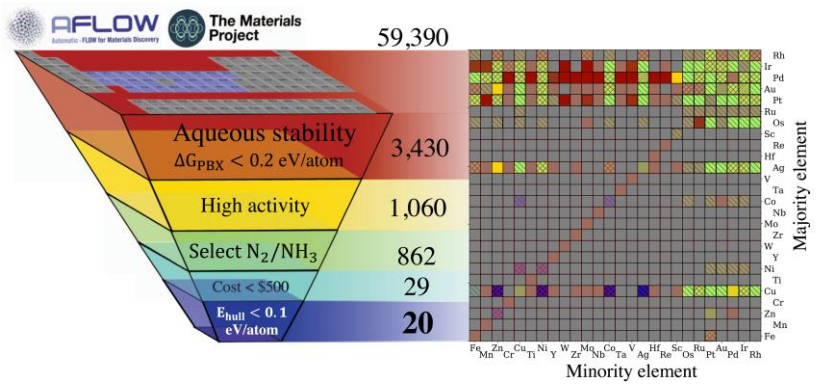
https://hackingmaterials.lbl.gov

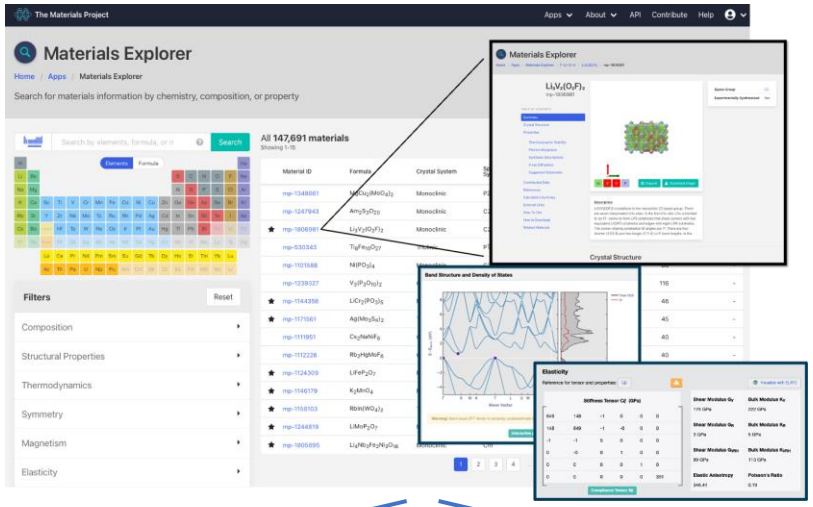
Acknowledgements:
Kristin Persson (Materials Project), Gerbrand Ceder (A-lab)

Quantum calculations (DFT) can predict the properties of new functional materials





Data can be combined into materials databases for design and machine learning



- The Materials Project (www.materialsproject.org)
- Free resource of calculated and contributed materials properties
- >150,000 inorganic compounds
- >250,000 registered users
- Most popular database for downstream machine learning (composition or structure → property)

MP for phosphors

Prediction
Statistical analysis of existing materials that co-occur with word 'phosphor' followed by structure prediction for new materials

Experiment
Predicted first known Sr-Li-Al-N quaternary, showed green-yellow/blue emission with quantum efficiency of 25% (Eu), 40% (Ce), 55% (co-activated Eu, Ce)

Sr_2LiAlN_4

References
- Wang, Z. et al. Mining Unexplored Chemistries for Phosphors for High-Color-Quality White-Light-Emitting Diodes. Joule 2, 914–926 (2018)
- Li, S. et al. Data-Driven Discovery of Full-Visible-Spectrum Phosphor. Chemistry of Materials 31, 6286–6294 (2019)
- Ha, J. et al. Color tunable single-phase Eu2+ and Ce3+ co-activated Sr2LiAlO4 phosphors. Journal of Materials Chemistry C 7, 7734–7744 (2019)

MP for carbon capture

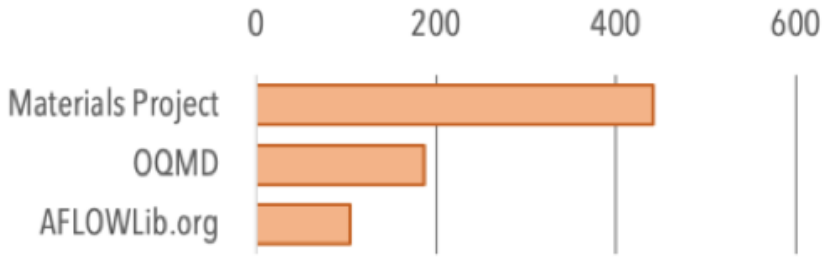
Prediction
Using phase diagram functionality, looked at 600 materials and 1400 carbonination reactions to extract 5 synthesis candidates

Experiment
Demonstration of rapid screening a success, with synthesized material demonstrating reversible carbonination

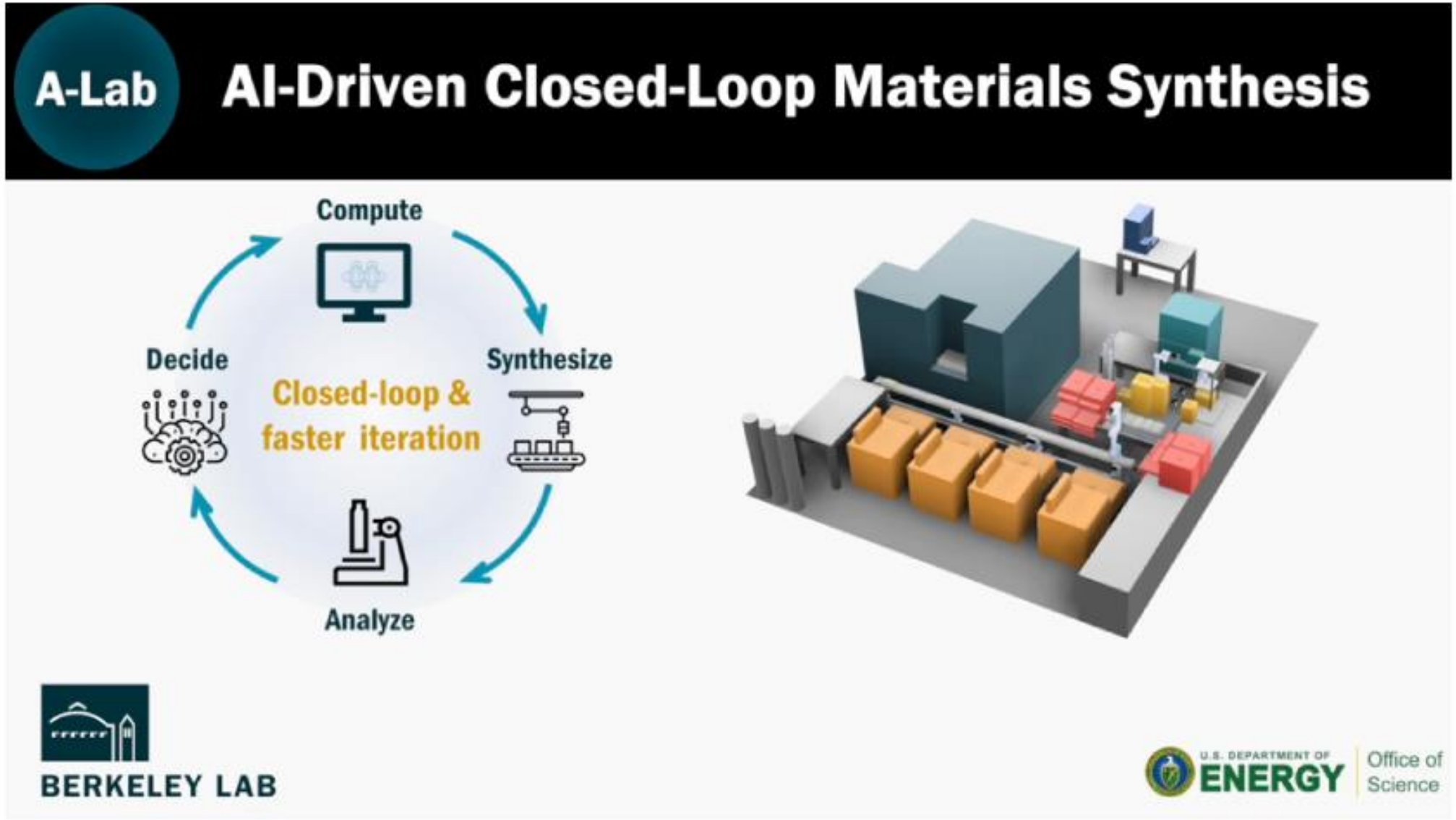
Na_3SbO_4

References
- Dunstan, M.T. et al. Large scale computational screening and experimental discovery of novel materials for high temperature CO2 capture. Energy & Environmental Science 9, 1346–1360 (2016).

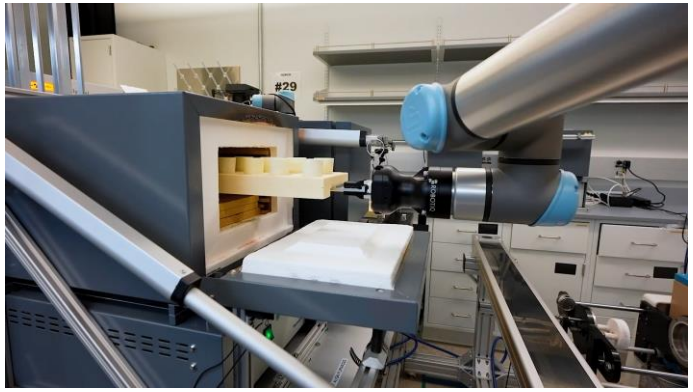
Databases cited by machine learning studies

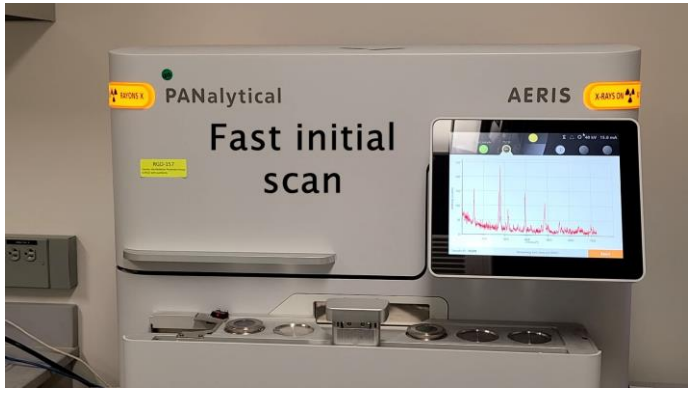


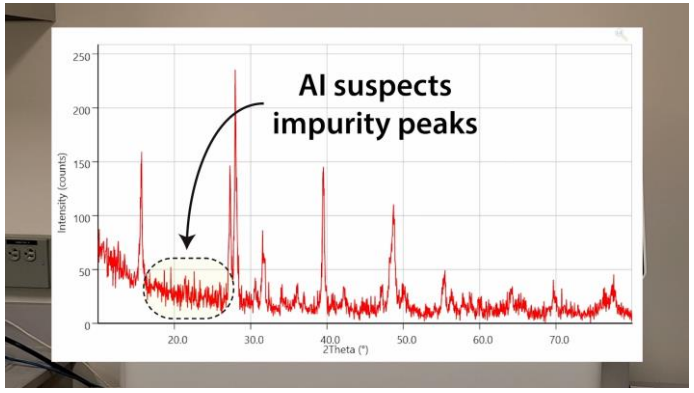
From the computer to the “A-lab” (video):

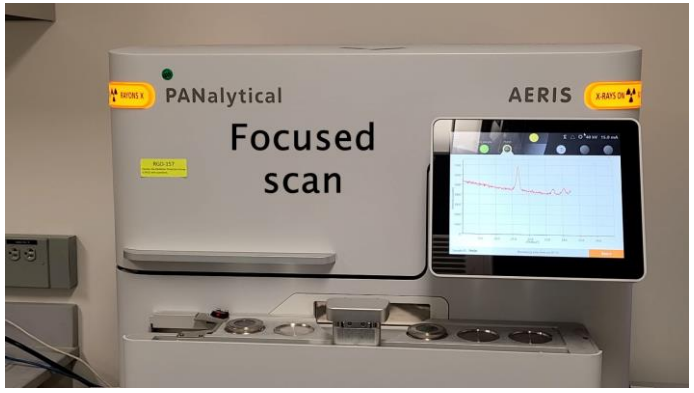


Szymanski, N. J. et al. An Autonomous Laboratory for the Accelerated Synthesis of Novel Materials. Nature 2023, 624 (7990), 86–91.




PANalytical
AERIS
Fast initial
scan


AI suspects
impurity peaks
Intensity (counts)
2Theta (°)


PANalytical
AERIS
Focused
scan