2018 Mission Innovation Workshop on

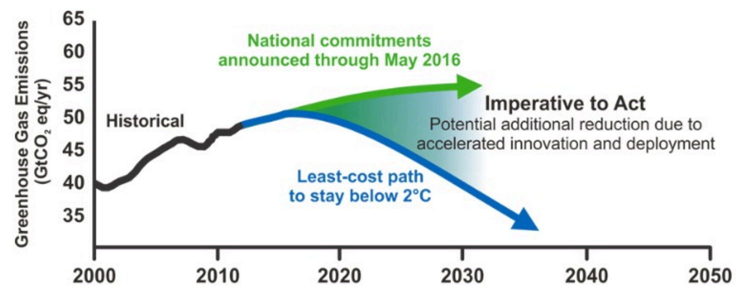
Materials Acceleration Platform: *Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence*

Joshua Schrier

Haverford College → Fordham University

MISSION INNOVATION
Accelerating the Clean Energy Revolution

- **Global** initiative
  - UN Climate Change Conference 2015 (Paris)
  - 23 Member Nations + European Union
    - (80% of global clean energy R&D Budget)
- **Goal**: Double government/state-directed clean energy R&D over five years.
  - Target: $30B USD/year in 2021
  - Private sector collaboration
- **http://mission-innovation.net**



Adapted from UNFCCC, Synthesis report of INDCs, May 2016

World leaders launch *Mission Innovation* at the United Nations Climate Change Conference 2015 (COP21) in Paris-Le Bourget, France, November 30, 2015.

Leaders supporting *Mission Innovation*, but not shown, are Park Geun-hye, President of the Republic of Korea; Stefan Löfven, Prime Minister of the Kingdom of Sweden; Angela Merkel, Chancellor of the Federal Republic of Germany; Malcolm Turnbull, Prime Minister of Australia.

Photo credit: Gobierno de Chile, "Ceremonia de lanzamiento de la Iniciativa "Mission Innovation", November 30, 2015, Creative Commons Attribution 2.0 Generic License.

Eight Innovation Challenges

		Australia	Austria	Brazil	Canada	Chile	China	Denmark	EC	Finland	France	Germany	India	Indonesia	Italy	Japan	Mexico	Norway	Republic of Korea	Saudi Arabia	Sweden	The Netherlands	UAE	UK	USA
1	Smart Grids Innovation Challenge	○	○	○	○		●	○	○	○	○	○	●	○	●		○	○	○	○	○	○		○	○
2	Off Grid Access to Electricity Innovation Challenge	○		○	○		○		○	○	●		●	○	○		○	○	○	○	○	○		○	○
3	Carbon Capture Innovation Challenge	○			○		○	○	○	○	○	○	○	○	○	○	●	○	○	●	○	○	○	●	○
4	Sustainable Biofuels Innovation Challenge	○		●	●	○	●		○	○	○		●	○	○		○	○			○	○		○	○
5	Converting Sunlight Innovation Challenge	○		○	○	○	○	○	●	○	○	●	○		○	○	○	○		○	○	○	○	○	○
6	Clean Energy Materials Innovation Challenge	○			●			○	○	○	○	○	○		○		●	○	○	○	○	○		○	○
7	Affordable Heating and Cooling of Buildings Innovation Challenge	○	○	○	○		○	○	●	○	○	○	○		○		○	○	○	○	○	○	●	●	○
8	Hydrogen Innovation Challenge	●	○		○		○		●		○	●	○		○	○		○		○				○	○

● Lead ○ Participant

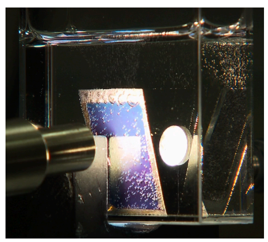
Materials are key for energy technology

Solar Energy

Wind Power

Gas separation and storage

Thermal energy conversion



Solar Fuels

Batteries

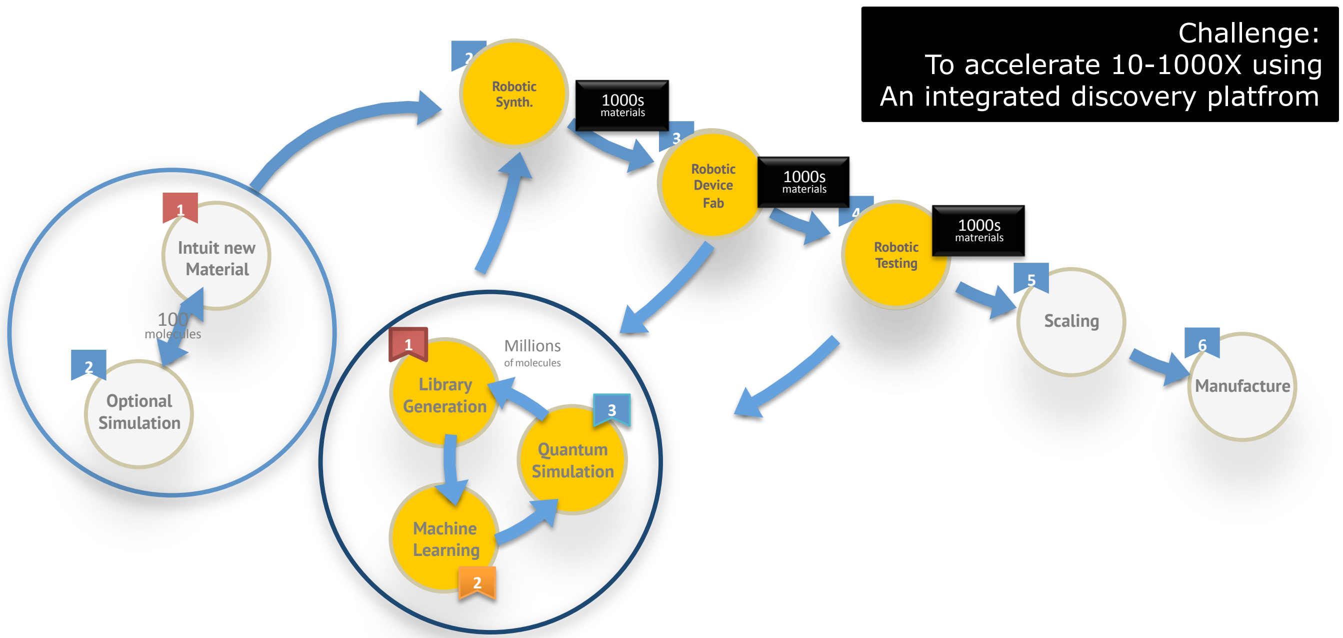
Power transmission

Eight Innovation Challenges

		Australia	Austria	Brazil	Canada	Chile	China	Denmark	EC	Finland	France	Germany	India	Indonesia	Italy	Japan	Mexico	Norway	Republic of Korea	Saudi Arabia	Sweden	The Netherlands	UAE	UK	USA
1	Smart Grids Innovation Challenge	Participant	Participant	Participant	Participant		Lead	Participant	Participant	Participant	Participant	Participant	Lead	Participant	Lead		Participant	Participant	Participant	Participant	Participant	Participant		Participant	Participant
2	Off Grid Access to Electricity Innovation Challenge	Participant		Participant	Participant		Participant		Participant	Participant	Lead		Lead	Participant	Participant		Participant	Participant	Participant	Participant	Participant	Participant		Participant	Participant
3	Carbon Capture Innovation Challenge	Participant			Participant		Participant	Participant	Participant	Participant	Participant	Participant	Participant	Participant	Participant	Participant	Lead	Participant	Participant	Lead	Participant	Participant	Participant	Lead	Participant
4	Sustainable Biofuels Innovation Challenge	Participant		Lead	Lead	Participant	Lead		Participant	Participant	Participant		Lead	Participant	Participant		Participant	Participant			Participant	Participant		Participant	Participant
5	Converting Sunlight Innovation Challenge	Participant		Participant	Participant	Participant	Participant	Participant	Lead	Participant	Participant	Lead	Participant		Participant	Participant	Participant	Participant		Participant	Participant	Participant	Participant	Participant	Participant
6	Clean Energy Materials Innovation Challenge	Participant			Lead			Participant	Participant	Participant	Participant	Participant	Participant		Participant		Lead	Participant	Participant	Participant	Participant	Participant		Participant	Participant
7	Affordable Heating and Cooling of Buildings Innovation Challenge	Participant	Participant	Participant	Participant		Participant	Participant	Lead	Participant	Participant	Participant	Participant		Participant		Participant	Participant	Participant	Participant	Participant	Participant	Lead	Lead	Participant
8	Hydrogen Innovation Challenge	Lead	Participant		Participant		Participant		Lead		Participant	Lead	Participant		Participant	Participant		Participant		Participant				Participant	Participant

Lead Participant

Mission Innovation Challenge 6:
Integrated materials design platform



SENER
SECRETARÍA DE ENERGÍA

ESTADOS UNIDOS MEXICANOS

CIFAR
CANADIAN INSTITUTE FOR ADVANCED RESEARCH

CONACYT
Consejo Nacional de Ciencia y Tecnología

Canada

MISSION INNOVATION
Accelerating the Clean Energy Revolution

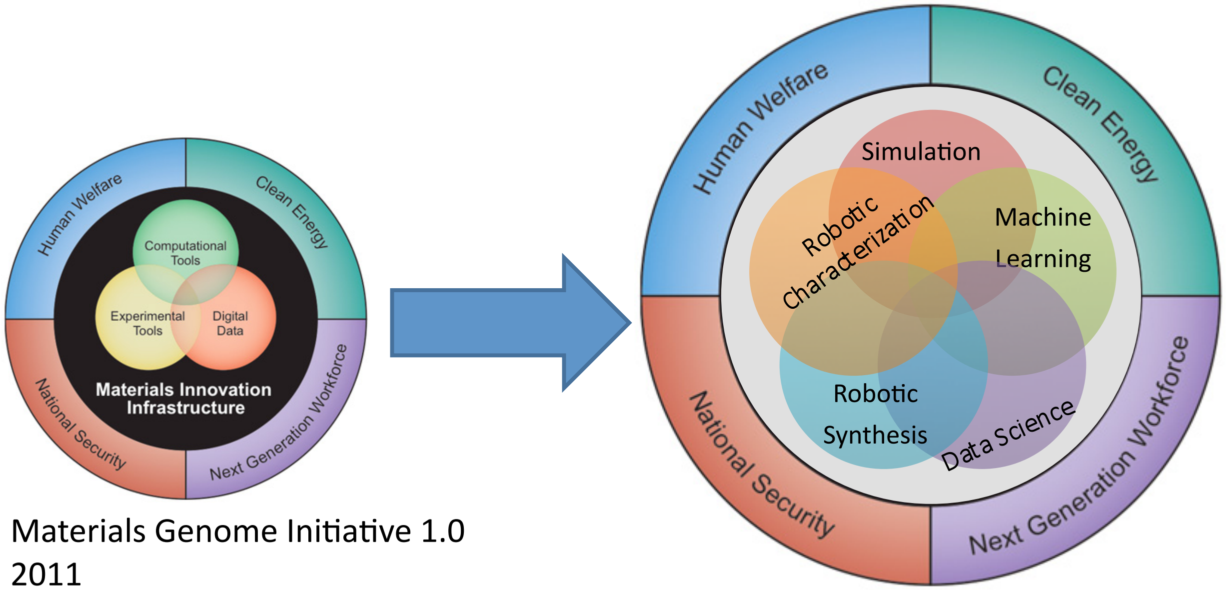
DEPARTMENT OF ENERGY UNITED STATES OF AMERICA

U.S. DEPARTMENT OF ENERGY

The workshop drew 133 attendees: *http://mission-innovation.net/2017/09/19/ic6-deep-dive-workshop/*

- 55 professors and scientists from top universities and research institutions;
- 6 keynote speakers and panellists, including Nobel Laureate Dr. Mario Molina;
- 16 MI member governments represented: Australia, Canada, Denmark, Finland, France, Germany, European Union, India, Italy, Korea, Mexico, Netherlands, Norway, Saudi Arabia, United Kingdom, and United States;
- affiliates of Mexico- and U.S.-based universities, groups, labs, and companies;
- graduate students and postdoctoral researchers; and observers from different countries

An integrated platform for materials discovery



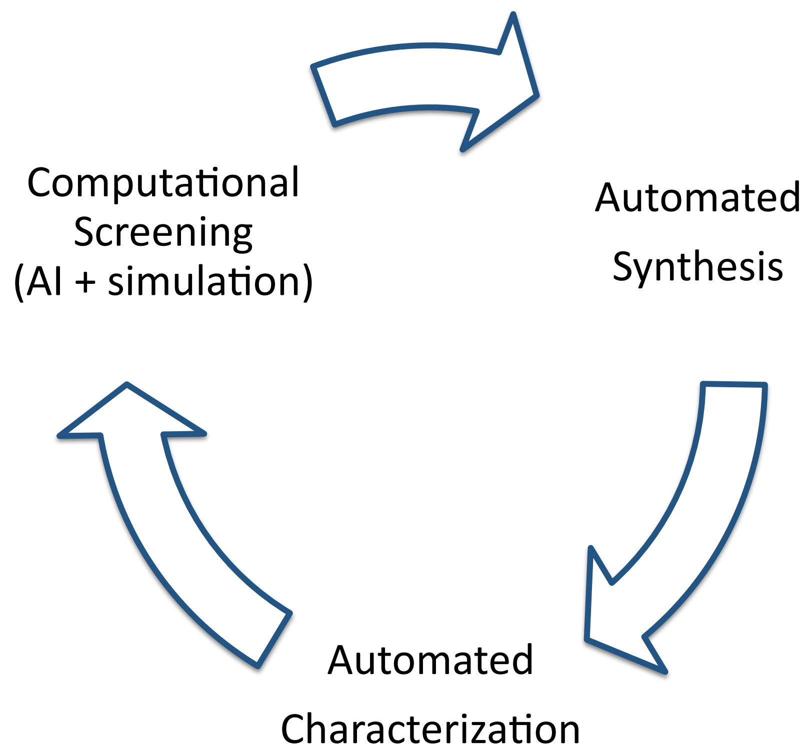
Materials Genome Initiative 1.0
2011

Mission Innovation Challenge 6
2017

Opportunity:
We need to strongly couple AI, robotics with computational materials genomics approaches
A "self-driving" laboratory is one possible goal

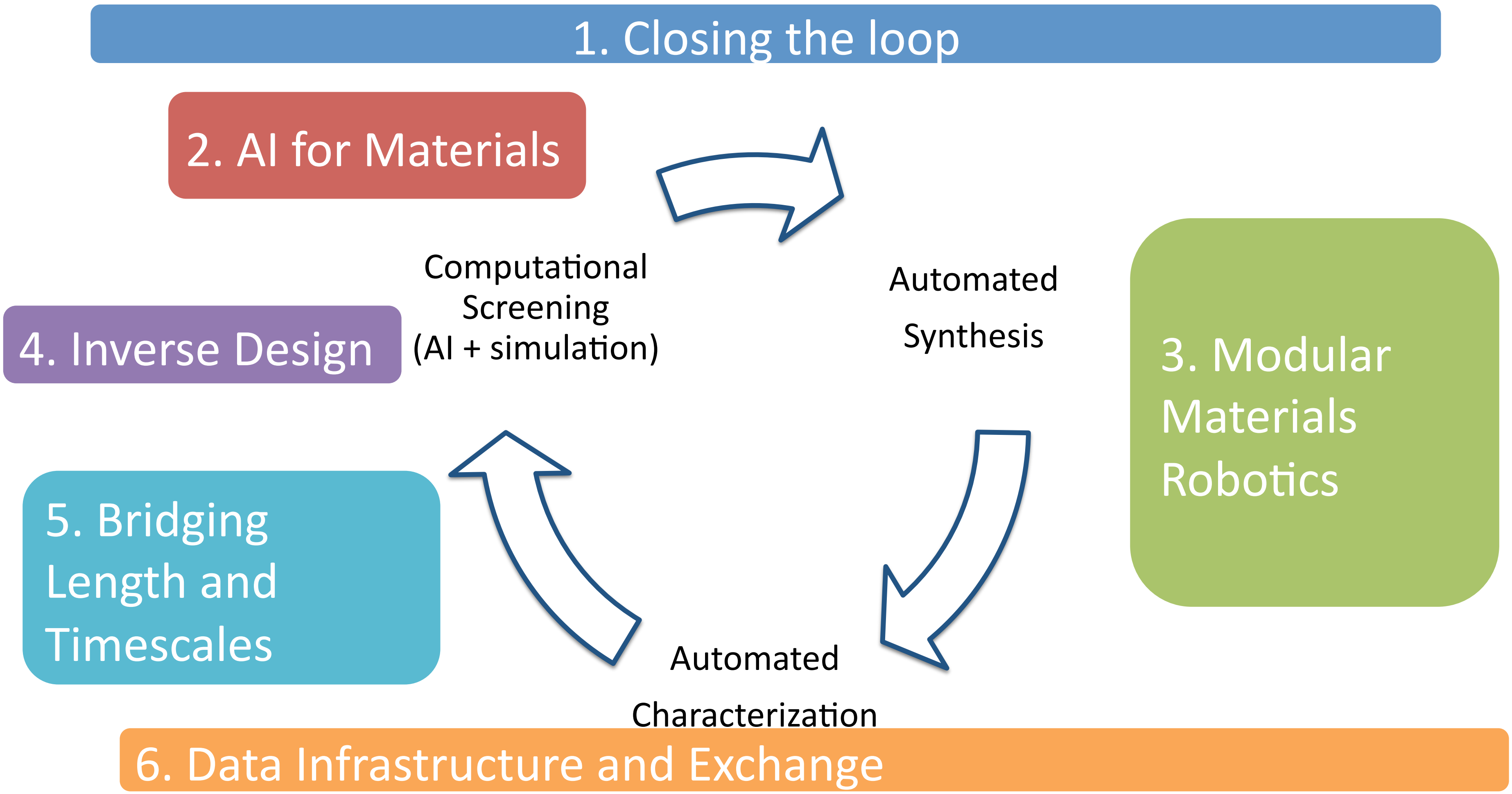
Materials Acceleration Platforms (MAPs)

Workshop's main recommendation



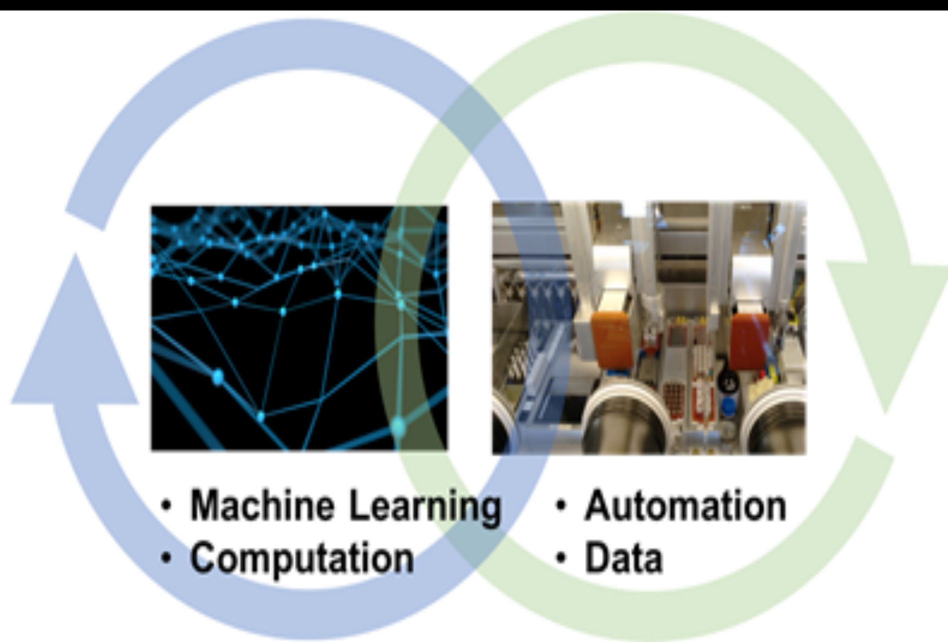
MAP elements

1. Closing the loop
2. AI for Materials
3. Modular Materials Robotics
4. Inverse Design
5. Bridging Length and Timescales
6. Data Infrastructure and Exchange


1. Closing the loop
2. AI for Materials
Computational
Screening
(AI + simulation)
Automated
Synthesis
3. Modular
Materials
Robotics
4. Inverse Design
5. Bridging
Length and
Timescales
Automated
Characterization
6. Data Infrastructure and Exchange

1. Closing the loop

Integrate powerful, yet usually separate elements of materials design, synthesis, and characterization in a closed loop.



1. Closing the loop

npj Computational Materials

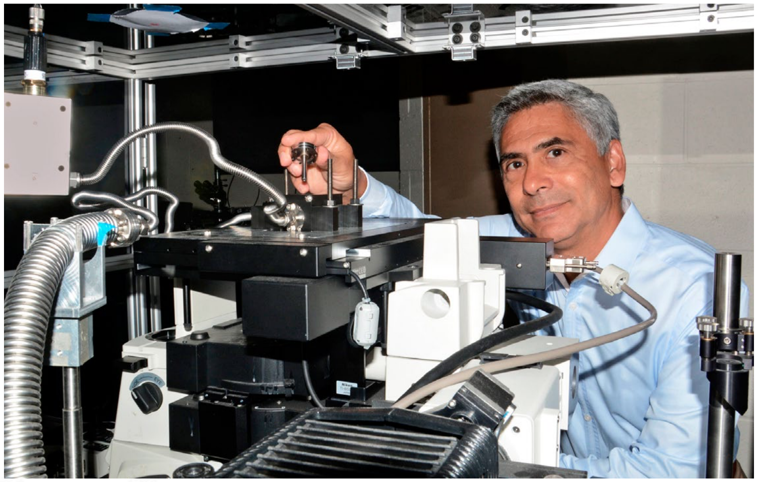
ARTICLE OPEN

Autonomy in materials research: a case study in carbon nanotube growth

Pavel Nikolaev[1,2], Daylond Hooper[1,2,4], Frederick Webber[1,2,5], Rahul Rao[1,2], Kevin Decker[1,2], Michael Krein[3], Jason Poleski[3], Rick Barto[3] and Benji Maruyama[1]

Advances in materials are an important contributor to our technological progress, and yet the process of materials discovery and development itself is slow. Our current research process is human-centred, where human researchers design, conduct, analyse and interpret experiments, and then decide what to do next. We have built an Autonomous Research System (ARES)—an autonomous research robot capable of first-of-its-kind closed-loop iterative materials experimentation. ARES exploits advances in autonomous robotics, artificial intelligence, data sciences, and high-throughput and *in situ* techniques, and is able to design, execute and analyse its own experiments orders of magnitude faster than current research methods. We applied ARES to study the synthesis of single-walled carbon nanotubes, and show that it successfully learned to grow them at targeted growth rates. ARES has broad implications for the future roles of humans and autonomous research robots, and for human-machine partnering. We believe autonomous research robots like ARES constitute a disruptive advance in our ability to understand and develop complex materials at an unprecedented rate.

npj Computational Materials (2016) **2,** 16031; doi:10.1038/npjcompumats.2016.31; published online 21 October 2016



Benji Maruyama
Air Force Research Laboratories

2. AI for Materials

Angewandte Chemie 10.1002/ange.201705721

COMMUNICATION WILEY-VCH

Human vs Robots in the Discovery and Crystallization of Gigantic Polyoxometalates

Vasilios Duros[+], Jonathan Grizou[+], Weimin Xuan, Zied Hosni, De-Liang Long, Haralampos N. Miras and Leroy Cronin*

Abstract: *The discovery of new gigantic molecules formed by self-assembly using single crystal X-ray crystallography is a challenging endeavor as it combines two contingent events; first is the formation of a new molecule, and second its crystallization. Herein, we constructed a workflow that can be followed manually or by a robot to probe the envelope of both events and employed it in the chemical space of a new polyoxometalate cluster, namely $Na_6[Mo_{120}Ce_6O_{366}H_{12}(H_2O)_{78}]\cdot 200H_2O$ (1) which*

hand. We compare
screening process in
crystallization condition
how human experimen
compare their strateg
learning approach.

So far, work in
simulations and only

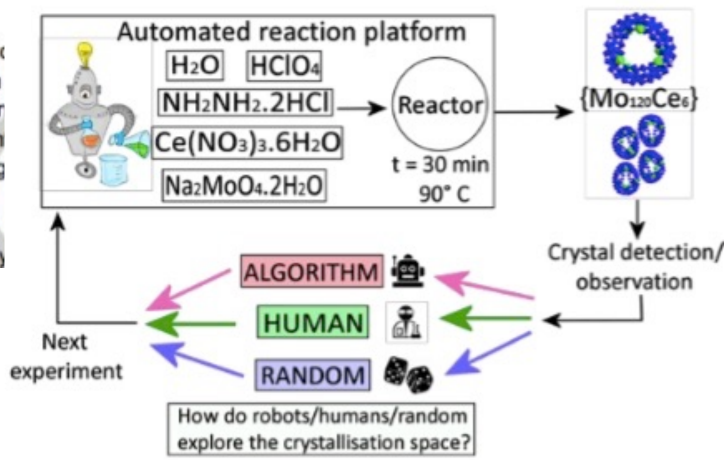
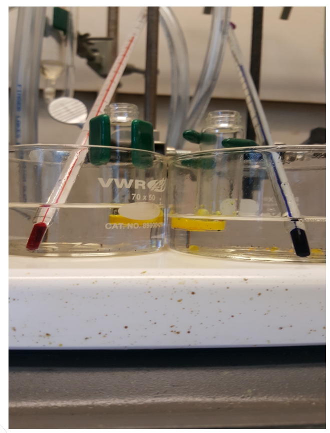


Figure 2. Representation of experimental protocol showing how the automated and bench work was done. Coloring code: Mo, blue; Ce, green. The different building units of $\{Mo_{120}Ce_6\}$ are represented with the same color for clarity.

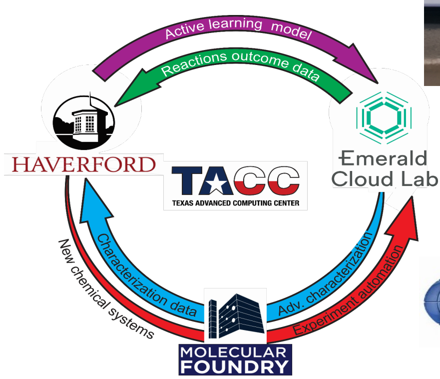
1. Closing the loop

Need: Digital experiment plans across diverse lab environments



Offline experiments
~20 reactions per day
(Haverford College)

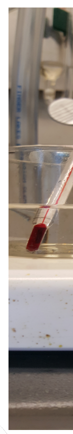
Semi-autonomous experiments
~200 reactions per day
(Molecular Foundry)

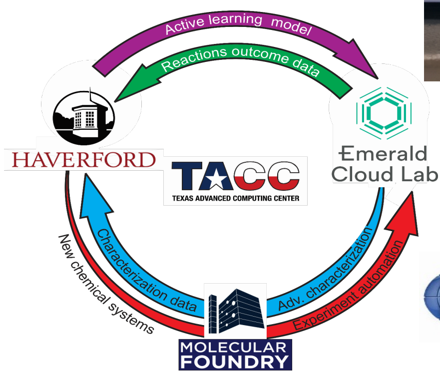


DARPA

1. Closing the loop

Need: Digital experiment plans across diverse lab environments





O
~2
(H

Fully-autonomous experiments
10^4 reactions per day
(Emerald Cloud Lab)

1. Closing the loop

Need: Programming language for experiments

```
In[ ]:= blue = Model[Sample, StockSolution, id:mnk9jOR3JNdm] (*1M Cu(II)SO4 aqueous solution, prepped on previous page*)
white = Model[Sample, Chemical, "Milli-Q water"]
red = Model[Sample, StockSolution, "Red Food Dye Test Solution"]

blueWells = Transpose[{
   (Join[
      AllWells["A1", "A5"], AllWells["B1", "B5"], AllWells["C1", "C5"], AllWells["D1", "D5"]] // Flatten),
   Table[200 - i, {i, 0, 19}]}]

redWells = Join[
   AllWells["A6", "A12"], AllWells["C6", "C12"], AllWells["E1", "E12"],
   AllWells["G1", "G12"]] // Flatten

whiteWells = Transpose[{
   Complement[Flatten[AllWells[]], blueWells[[All, 1]]] (*dilute the red wells*),
   Table[80 + i, {i, 96 - 20}]}]
```

1. Closing the loop

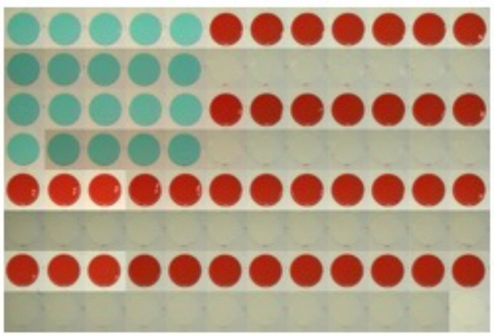
Need: Programming language for experiments

```
flagExperiment2 = ExperimentSampleManipulation[
  {flagPlate = Model[Container, Plate, "96-well UV-Star Plate"]}, (*compatible with UV/vis*)
  (
   Join[
    Transfer[
       Source → blue, Amount → #[[2]] Micro Liter, Destination → {flagPlate, #[[1]]}] & /@ blueWells,
    Transfer[
       Source → red, Amount → 20 Micro Liter, Destination → {flagPlate, #}] & /@ redWells,
    Transfer[
       Source → white, Amount → #[[2]] Micro Liter, Destination → {flagPlate, #[[1]]}] & /@ whiteWells
   ]
  ),
  ImageSample → True
 ]
ExperimentImageSample[flagExperiment2[ContainersOut] // First]
ExperimentMeasureVolume[flagExperiment2[ContainersOut] // First, Method → Ultrasonic],
ExperimentAbsorbanceSpectroscopy[flagExperiment2[ContainersOut] // First, ImageSample → True]
```

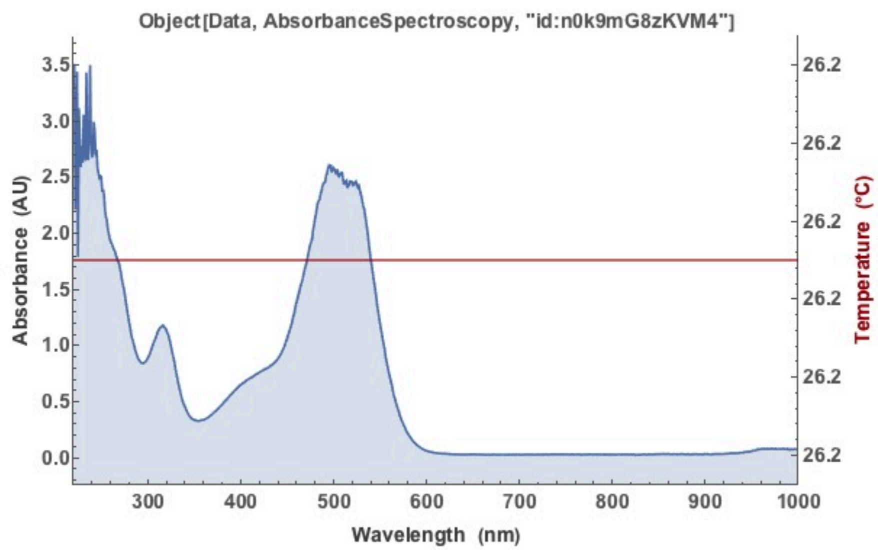
1. Closing the loop

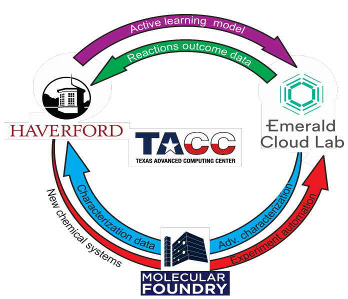
Need: Programming language for experiments

```
ImageAssemble[Partition[(ImageTake[#, {20, 50}, {30, 60}] &/@ sortedImages), 12]]
```

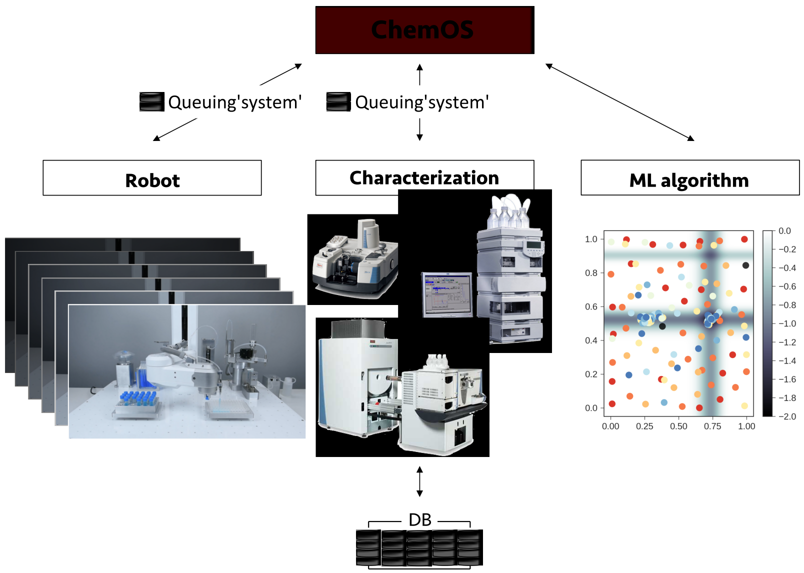


```
Object[Protocol, AbsorbanceSpectroscopy, "id:AEqRl9K5dwAv"][Data][[21]] // PlotAbsorbanceSpectroscop
```





2. AI for Materials



AI-controlled chemical laboratory
Jason Hein, University of British Columbia
Alan Aspuru-Guzik, Harvard University

Autonomous research relies on reasoning, decision making, and creativity.

The particular scale and details of theoretical, computational, synthetic, and characterization evidence in materials research require the establishment of this new branch of AI.

National and international research organizations must facilitate an integrated computer and materials science research effort to develop algorithms that mimic, and then supersede, the intellect and intuition of expert materials scientists.

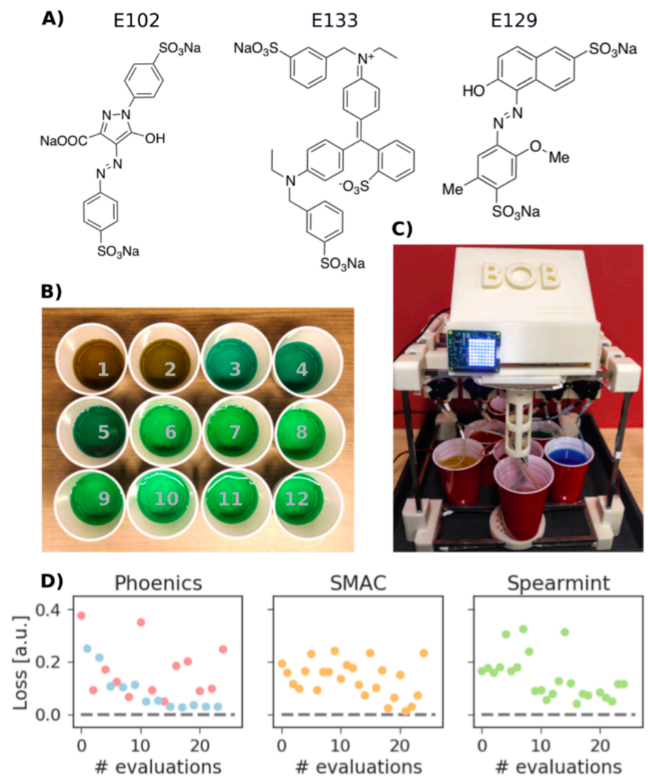
ChemOS: an orchestration software to democratize autonomous discovery

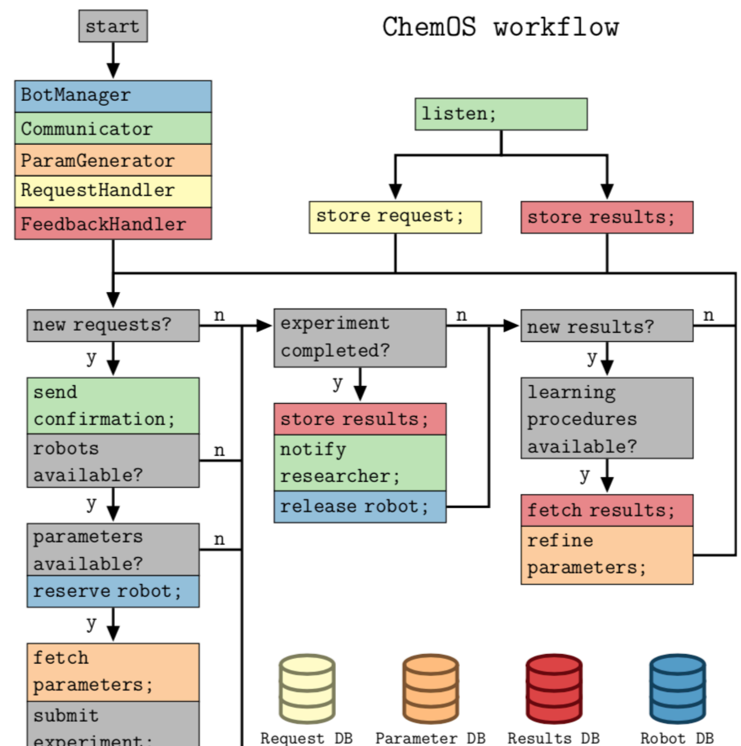
Loïc M. Roch,[1, a)] Florian Häse,[1, a)] Christoph Kreisbeck,[1] Teresa Tamayo-Mendoza,[1] Lars P. E. Yunker,[2] Jason E. Hein,[2] and Alán Aspuru-Guzik[1, 3, b)]

[1)] *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, 02138, USA*

[2)] *Department of Chemistry, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada*

[3)] *Senior Fellow, Canadian Institute for Advanced Research, Toronto, Ontario M5G 1Z8, Canada*





Roch, et al. **ChemRXiv:5953606 (2018)**

2. AI for Materials

ACS central science

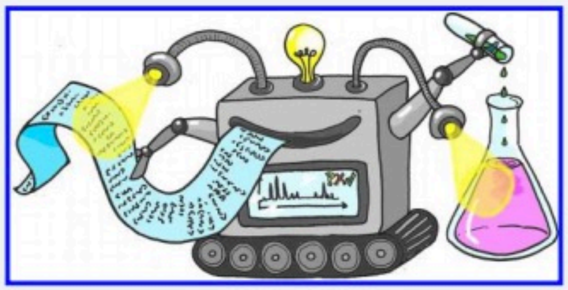
Outlook

Cite This: ACS Cent. Sci. XXXX, XXX, XXX–XXX

Designing Algorithms To Aid Discovery by Chemical Robots

Alon B. Henson, Piotr S. Gromski, and Leroy Cronin*

WestCHEM, School of Chemistry, University of Glasgow, Glasgow G12 8QQ, United Kingdom

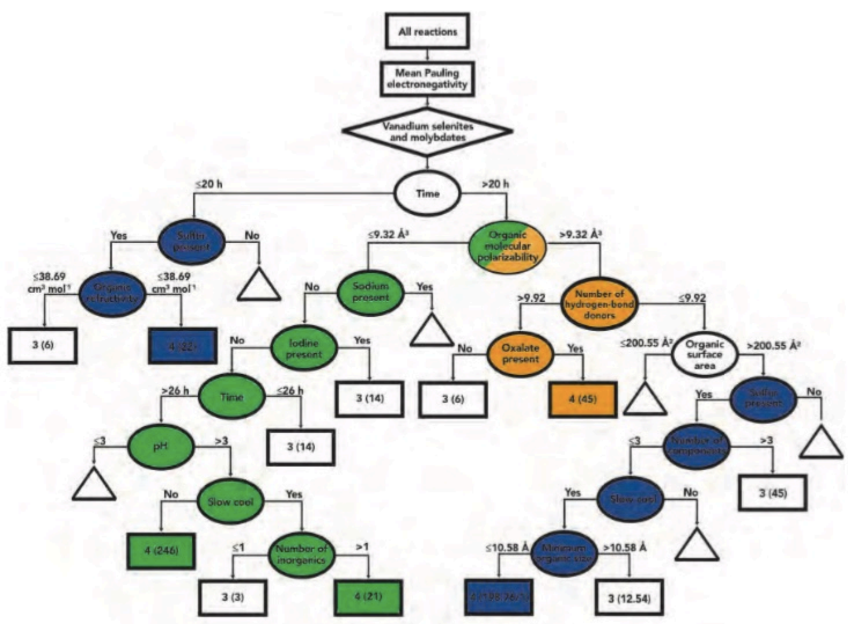


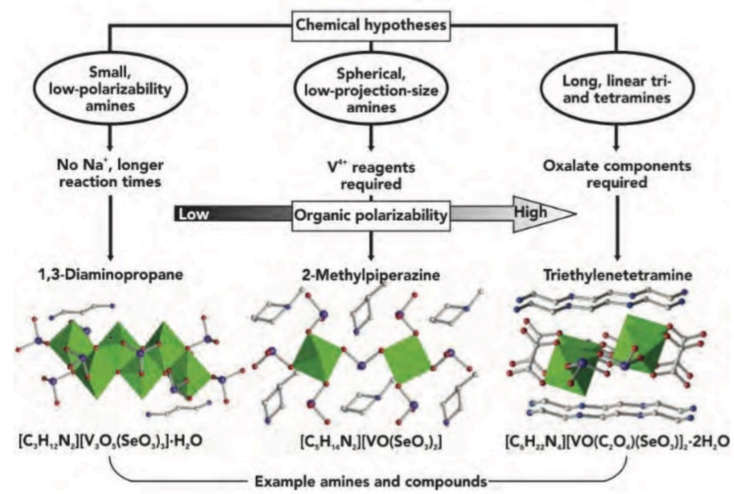
ABSTRACT: Recently, automated robotic systems have become very efficient, thanks to improved coupling between sensor systems and algorithms, of which the latter have been gaining significance thanks to the increase in computing power over the past few decades. However, intelligent automated chemistry platforms for discovery orientated tasks need to be able to cope with the unknown, which is a profoundly hard problem. In this Outlook, we describe how recent advances in the design and application of algorithms, coupled with the increased amount of chemical data available, and automation and control systems may allow more productive chemical research and the development of chemical robots able to target discovery. This is shown through examples of workflow and data processing with automation and control, and through the use of both well-used and cutting-edge algorithms illustrated using recent studies in chemistry. Finally, several algorithms are presented in relation to chemical robots and chemical intelligence for knowledge discovery.

Cronin & co. DOI: 10.1021/acscentsci.8b00176

2. AI for Materials

Importance of interpretability—”machine rhetoric”

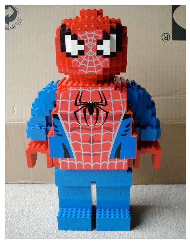


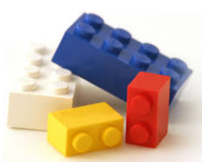


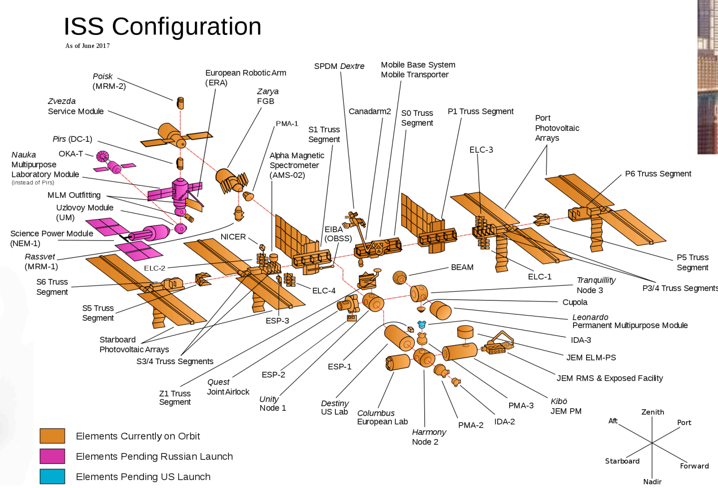
Friedler, Norquist, Schrier DOI: 10.1038/nature17439

How can we achieve exponential efficiency growth?

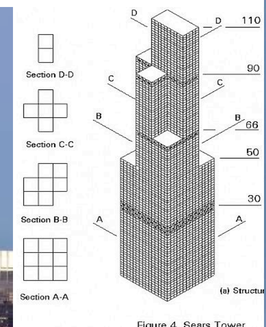
To achieve scale, use a modular approach





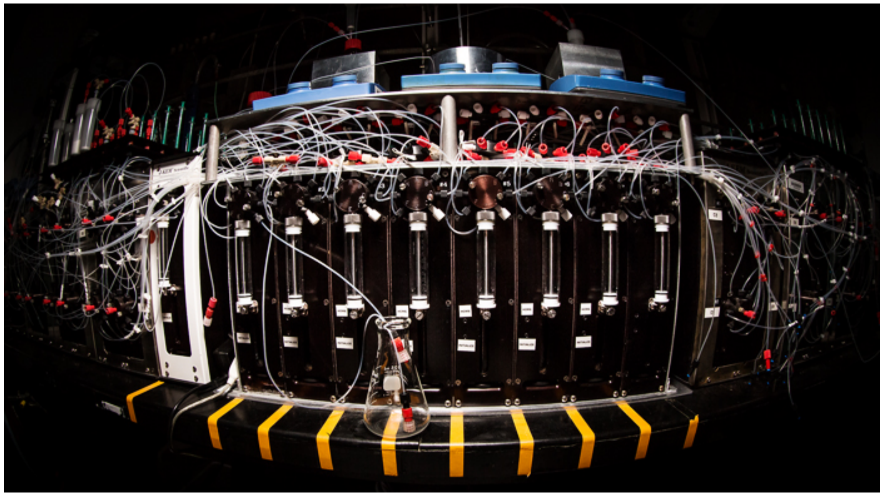


Sears Tower



Burj Khalifa

3. Modular Materials Robotics



The Synthesis Machine
Marty Burke, University of Illinois at Urbana Champaign

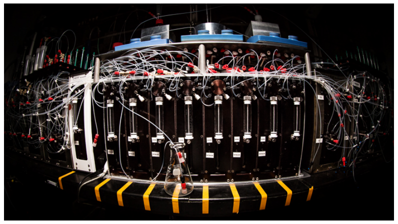
Autonomous laboratories must remain nimble and motivate a modular approach to the development of materials science automation.

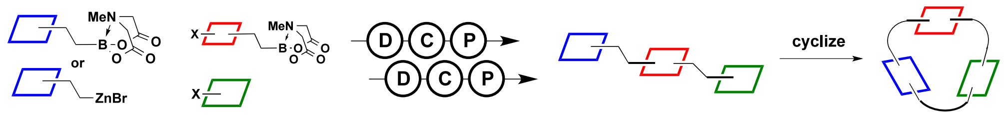
Representing techniques and materials as modular “building blocks” fosters human-machine communication and simplifies materials exploration.

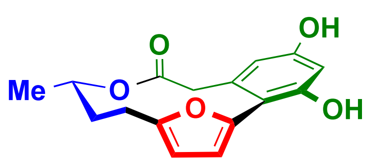
The Synthesis Machine

Marty Burke, University of Illiniois at Urbana Champaign

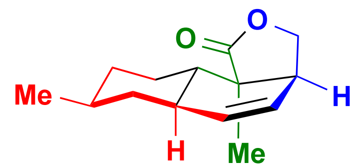
3. Modular Materials Robotics



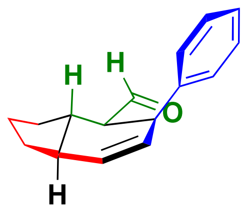




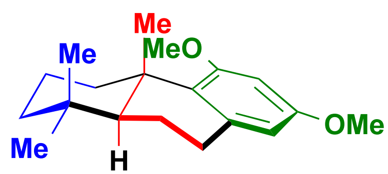
citreofuran



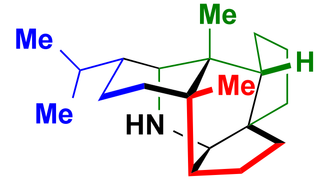
oblongolide



hexahydroindene core



steroid-like core



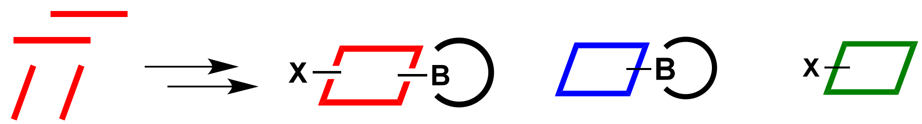
(±)-secodaphnane core

Burke et al *Science* **2015**, *347*, 1221-1226

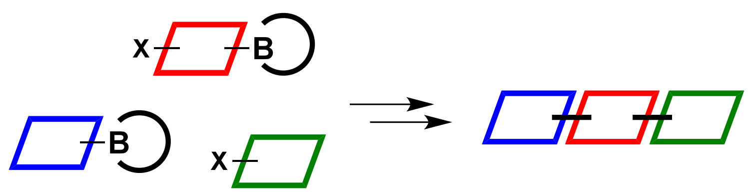
A similar approach for materials

Sequence

Build



Assemble



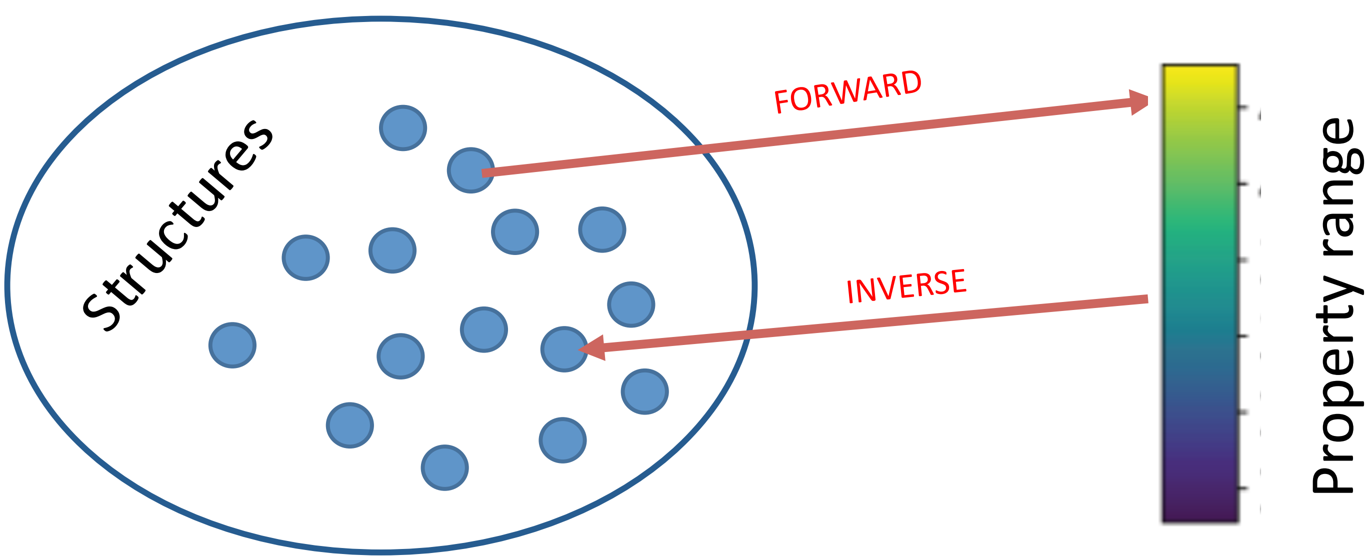
Burke et al *Science* **2015**, *347*, 1221-1226

The Synthesis Machine
Marty Burke, University of Illinois at Urbana Champaign

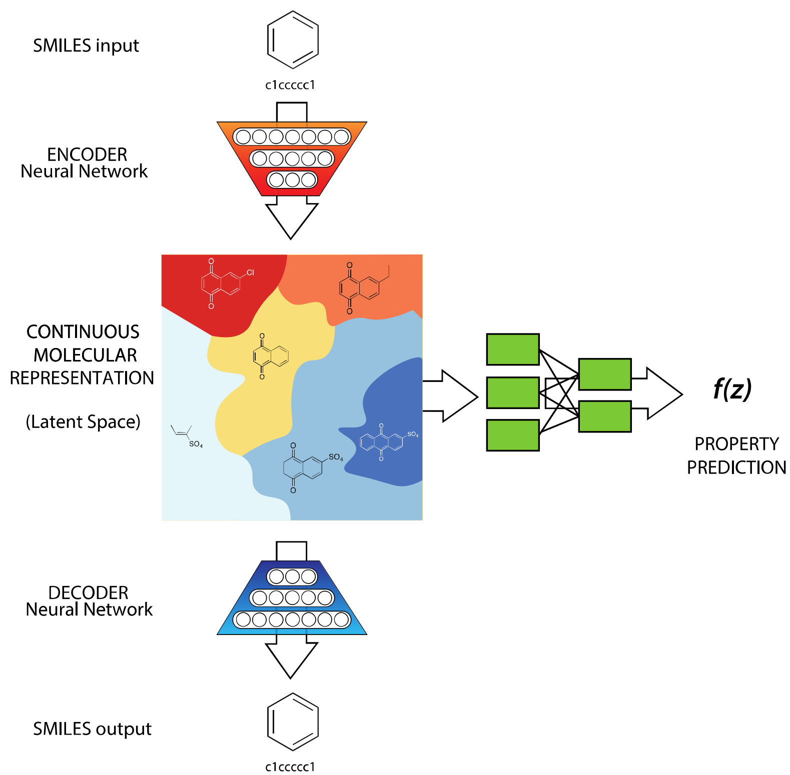
3. Modular Materials Robotics

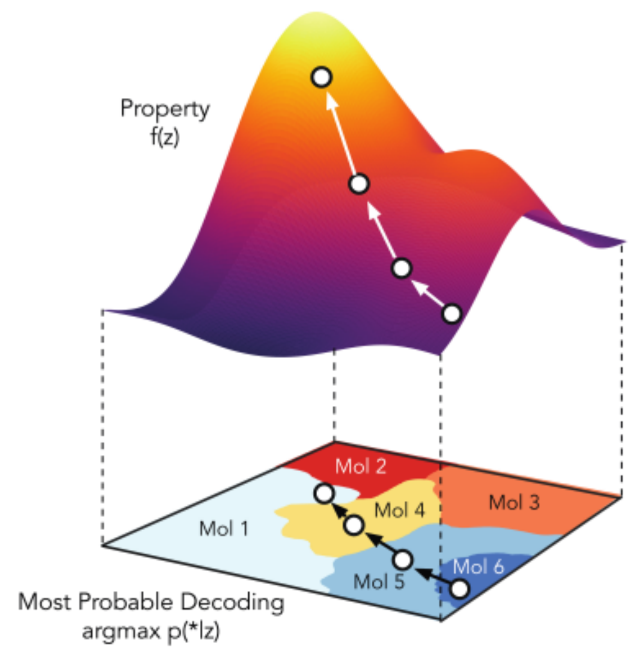
4. Inverse Design

Inverse design enables automated generation of candidate materials designed to meet the performance, cost, and compatibility requirements of a given clean energy technology.



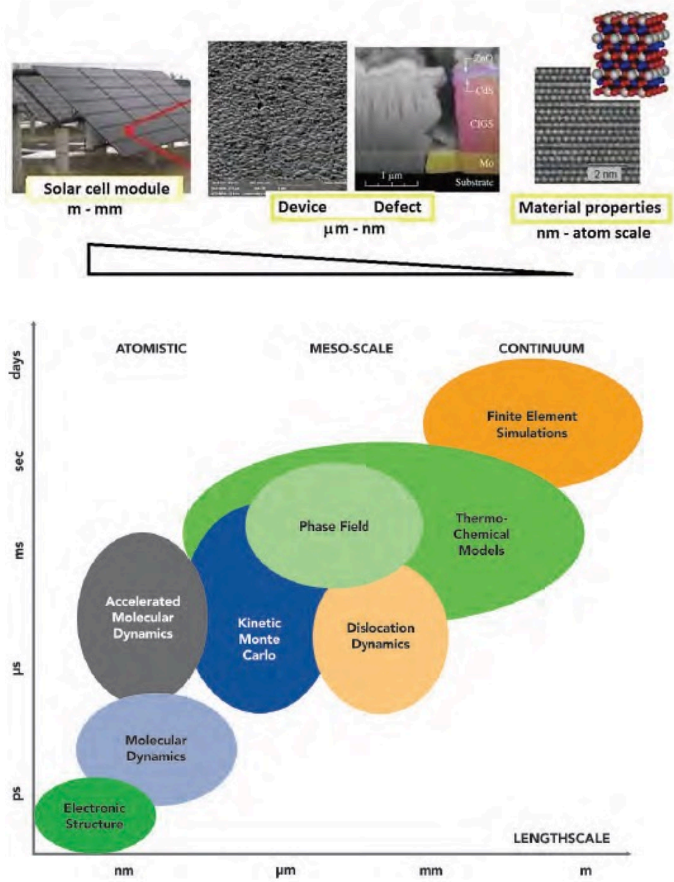
Autoencoders for chemical space





R. Gomez-Bombarelli, et al ACS Central Science (2018) 10.1021/acscentsci.7b00572

5. Bridging Length and Timescales



Materials systems frequently demand understanding and control of properties that span 10-orders of magnitude ranges of length and time scales.

Existing experimental and computational methods provide a view of a small part of this range.

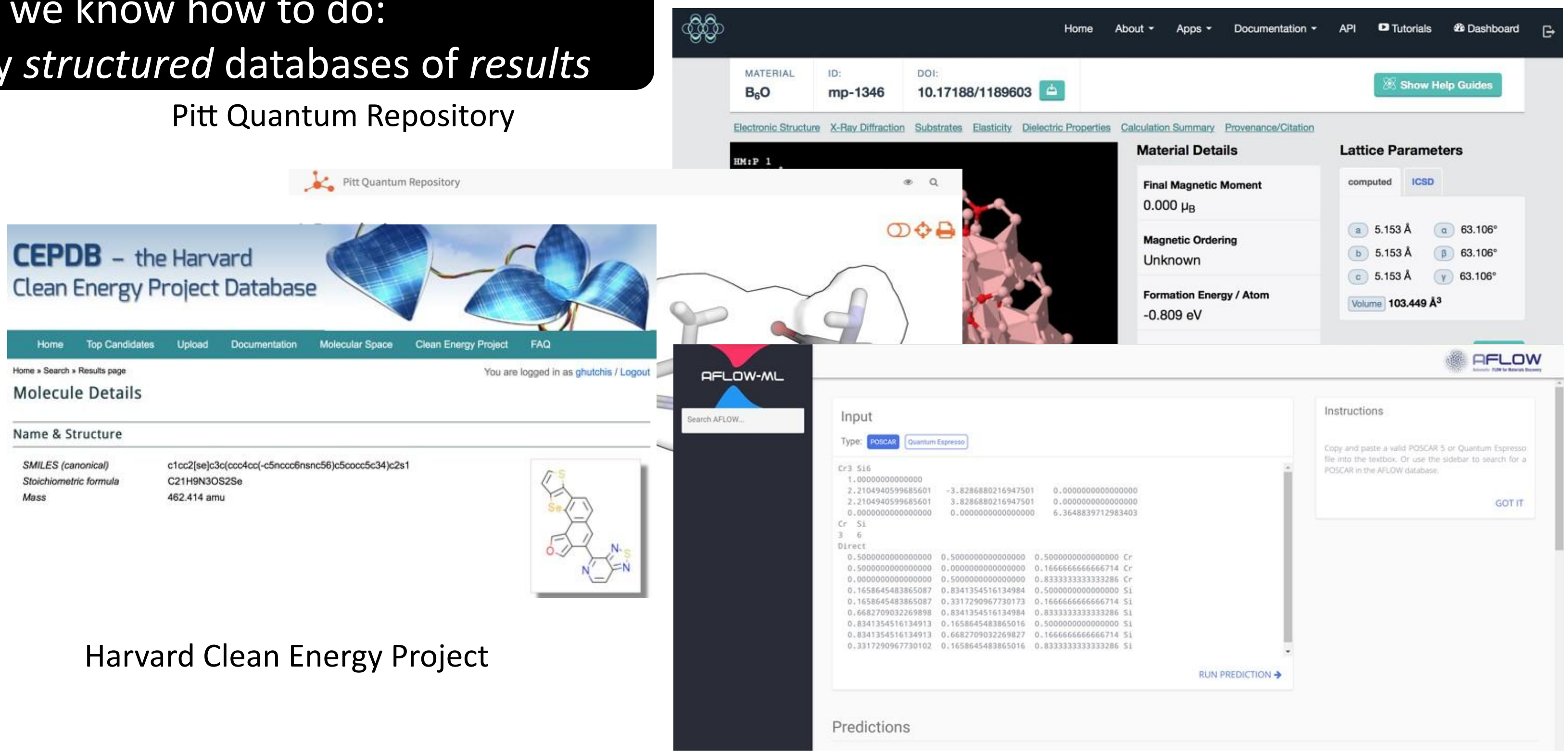
Propose:
ML as the “glue” between these methods—replace human expertise.

6. Data Infrastructure and Exchange

What we know how to do:
Highly *structured* databases of *results*

The Materials Project

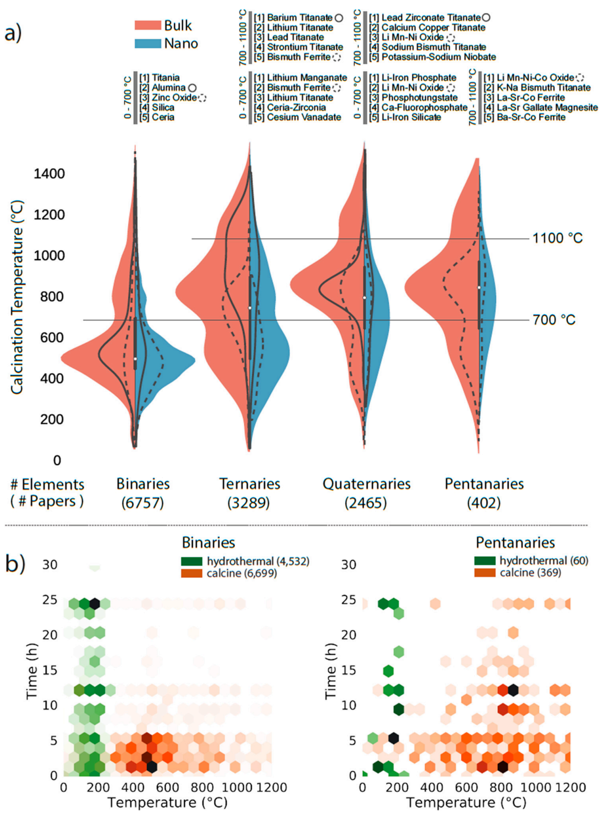
Pitt Quantum Repository



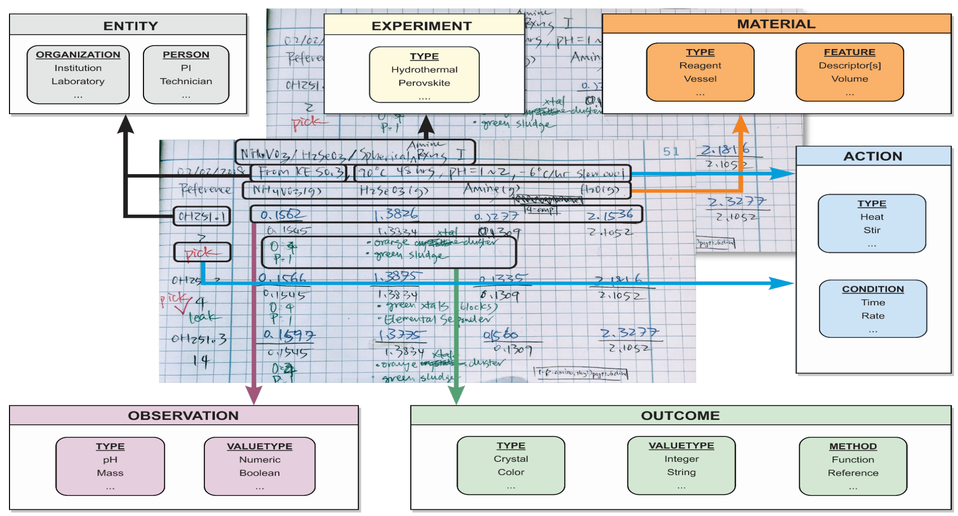
Harvard Clean Energy Project

AFLOW-lib and AFLOW-ml

6. Data Infrastructure and Exchange

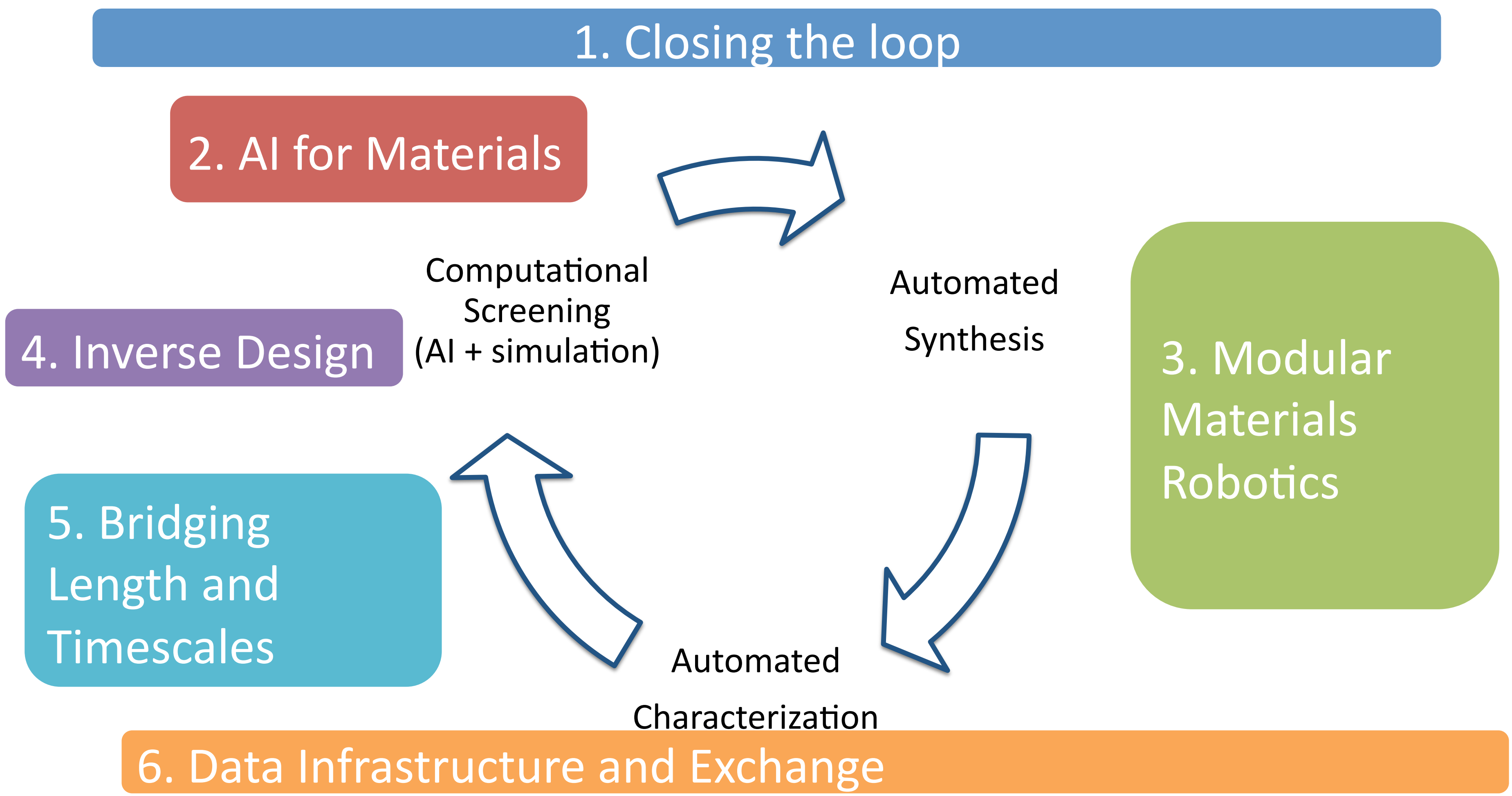


Challenge:
Extracting data from unstructured natural language sources—literature, lab notebooks, “dark” reactions



E. Olivetti @ MIT DOI: 10.1021/acs.chemmater.7b03500

Friedler, Norquist, Schrier DOI: 10.1038/nature17439


1. Closing the loop
2. AI for Materials
Computational
Screening
(AI + simulation)
Automated
Synthesis
3. Modular
Materials
Robotics
4. Inverse Design
5. Bridging
Length and
Timescales
Automated
Characterization
6. Data Infrastructure and Exchange

Follow-up workshops

- **Expert Workshop: Structural Materials and 3D Printing**
  - (March 2018, Hamilton, Canada)
  - http://ic6-2.mission-innovation.net/
- **Industry Meeting: Self-Driving Materials Laboratories: The Next Paradigm for Accelerated Discovery**
  - (May 2018, Toronto)
  - http://ic6-3.mission-innovation.net/

Learn more!

http://mission-innovation.net/our-work/innovation-challenges/clean-energy-materials-challenge/

And download the report!


Thank you!
Questions?