ILP 2018 MIT Research and Development Conference

New Methodologies in Materials Research for Accelerated Innovation

Carl V. Thompson, Director, Materials Research Laboratory
Stavros Salapatos Professor of Materials Science and Engineering

- **The Materials Research Laboratory**
- **The Nature Materials Research**
- **New Methods and Methodologies**

MIT MATERIALS RESEARCH LABORATORY

Massachusetts Institute of Technology

The Materials Research Laboratory

https://mrl.mit.edu/

- **Promotes Interdisciplinary Materials Research**
- **Provides a Nexus for Internal and External Communication**
- **Engages with Industry**

MRL Industry Collegium; Partnering with ILP and MIT.nano

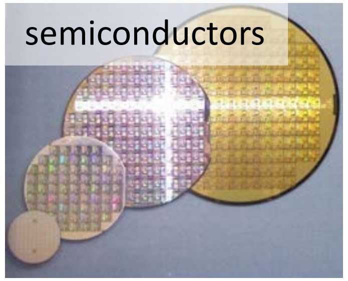
MIT MATERIALS RESEARCH LABORATORY

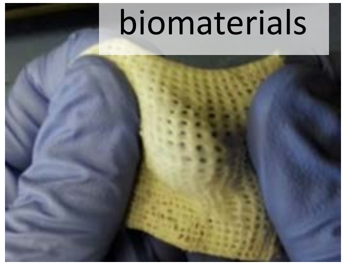
Massachusetts Institute of Technology

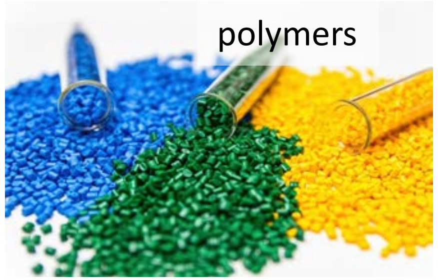
Materials for:

- Tissue engineering
- In vivo drug delivery
- Biomedical devices
- Batteries: metal-ion, flow, metal-air
- Solar cells
- Mechanical energy harvesting
- Thermal energy harvesting
- Hydrolysis
- Fuel cells
- Quantum computing
- Computation
- Sensing
- Water treatment
- Displays
- Coatings
- Catalysts
- Structures
- Transportation

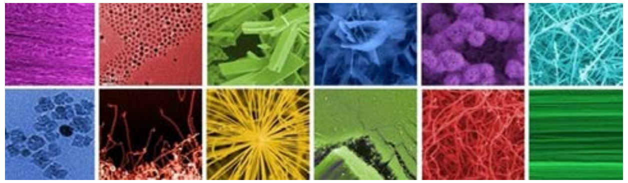
….. and more!





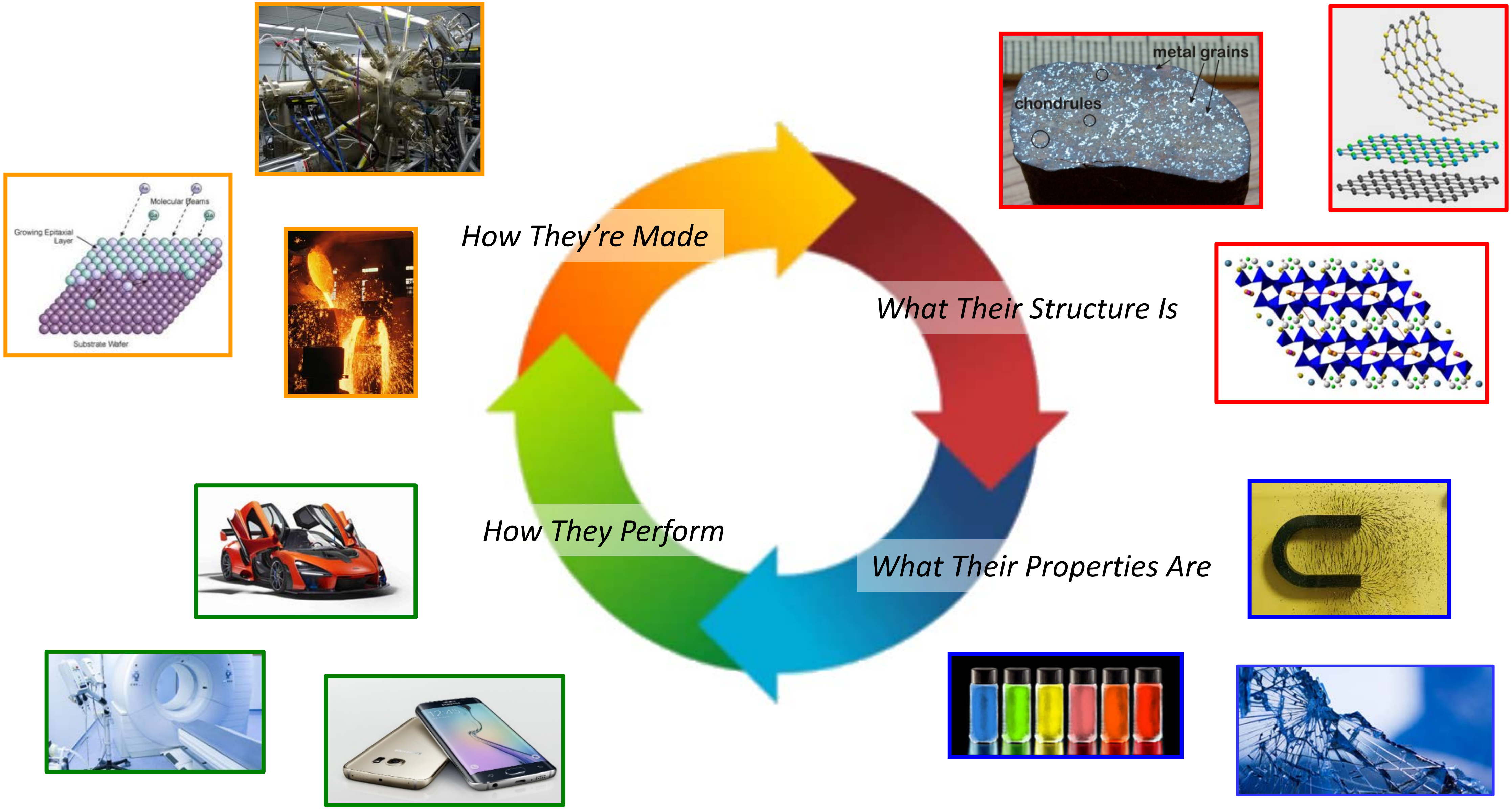


nanomaterials

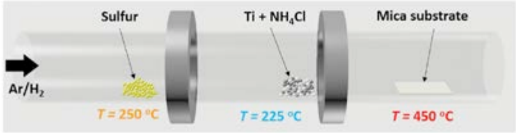


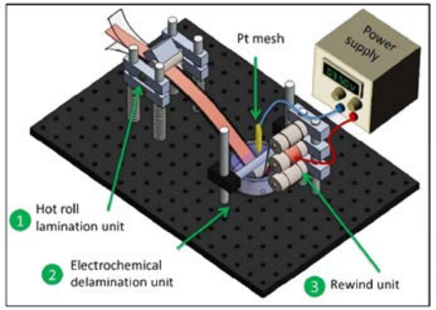
Over 150 faculty and their groups carry out materials research at MIT!

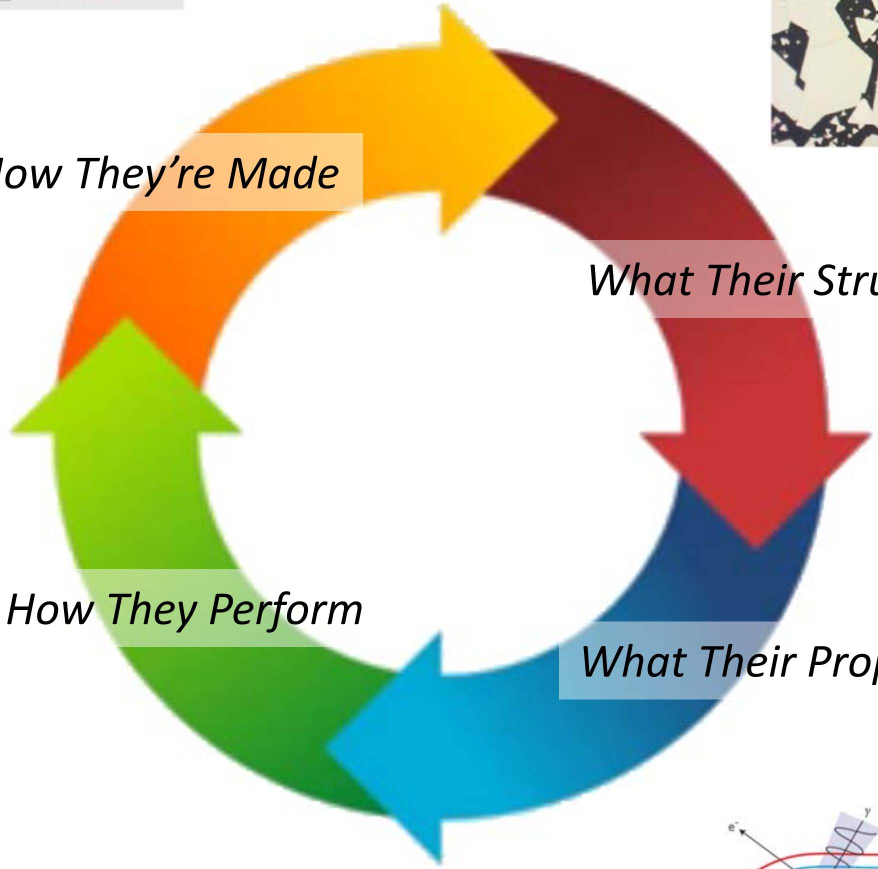
Materials Research

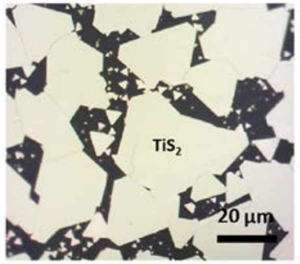


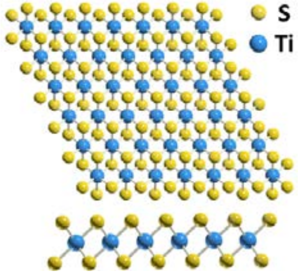
2D Materials Research

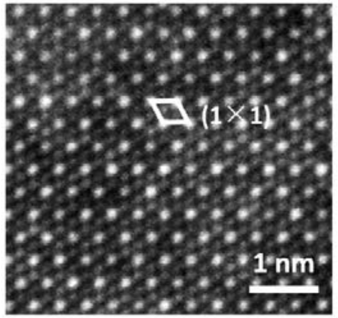


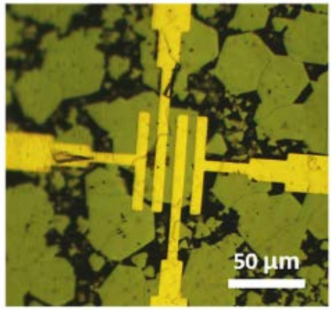


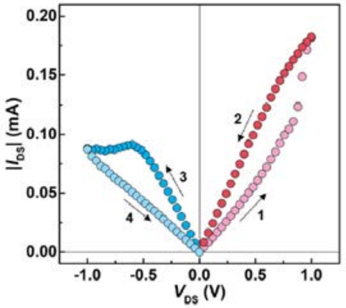




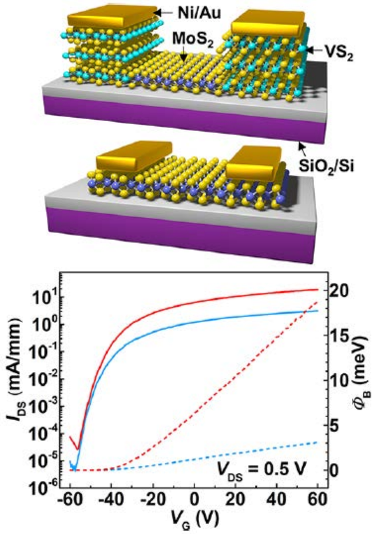




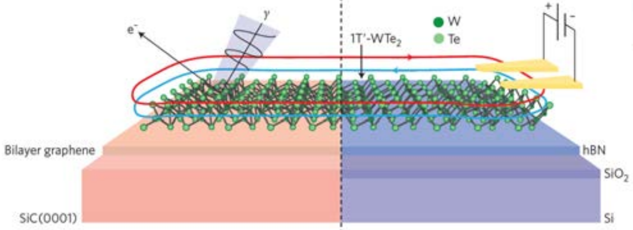




memristor

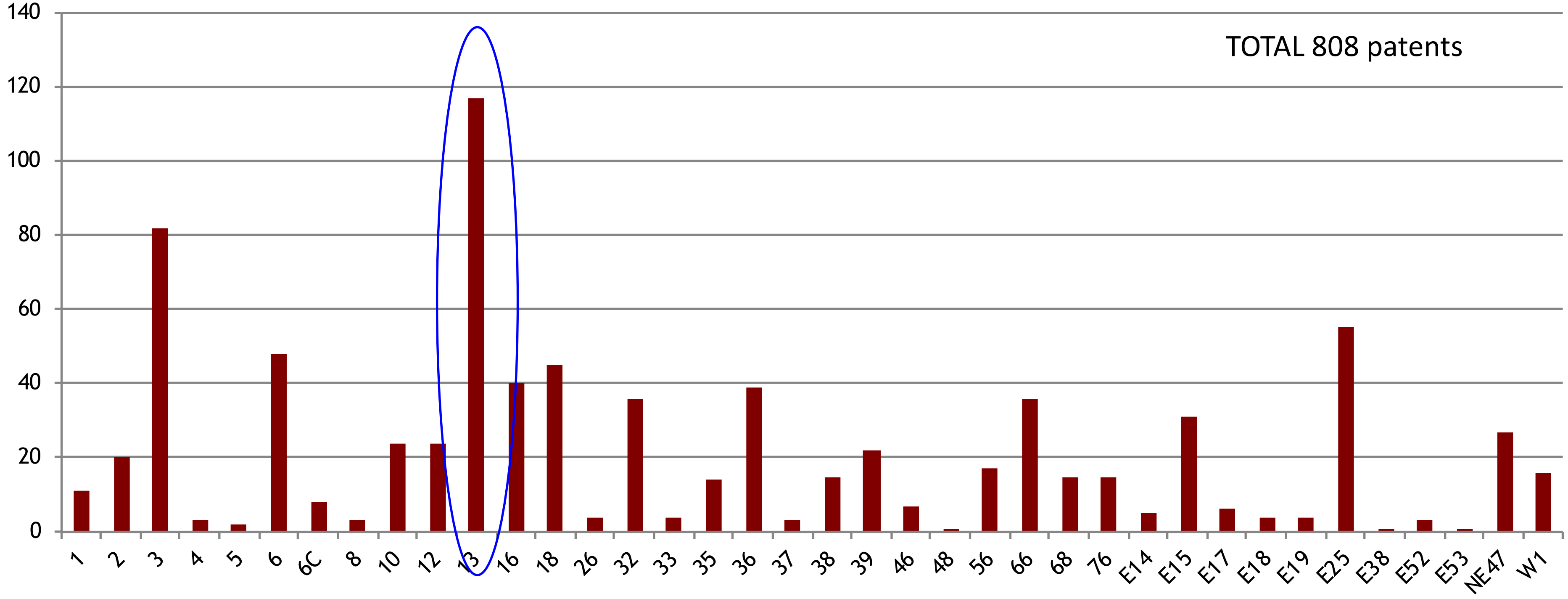


MOSFET



Patents issued to MIT Faculty by Building

(between 2005 and 2011)



MRL faculty have founded dozens of companies:

QD VISION

Photography by Felice Frankel

LUMINUS

microchips BIOTECH

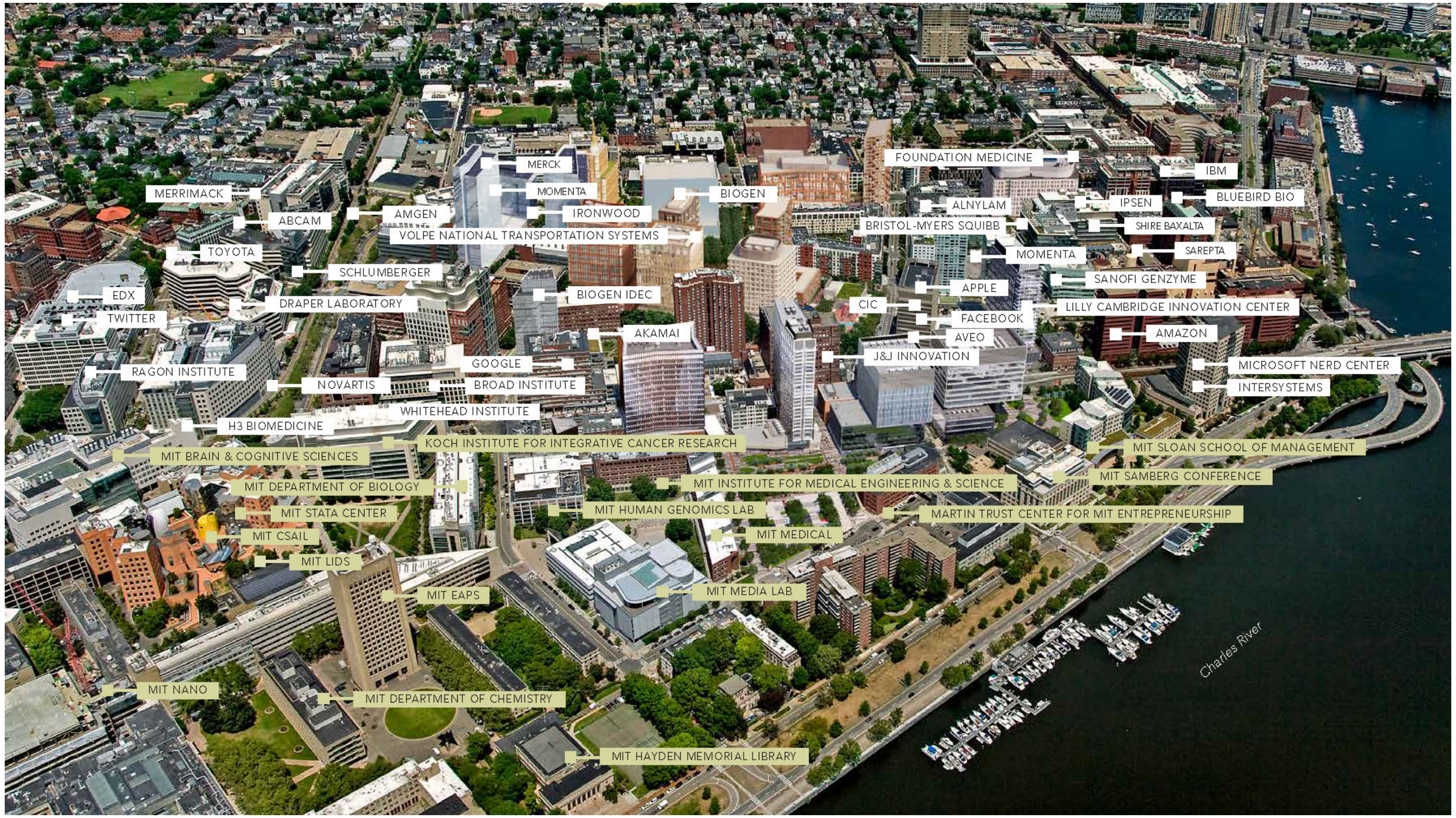
OmniGuide®

AmberWave

nanosys™

AMBRI

The Power of Proximity

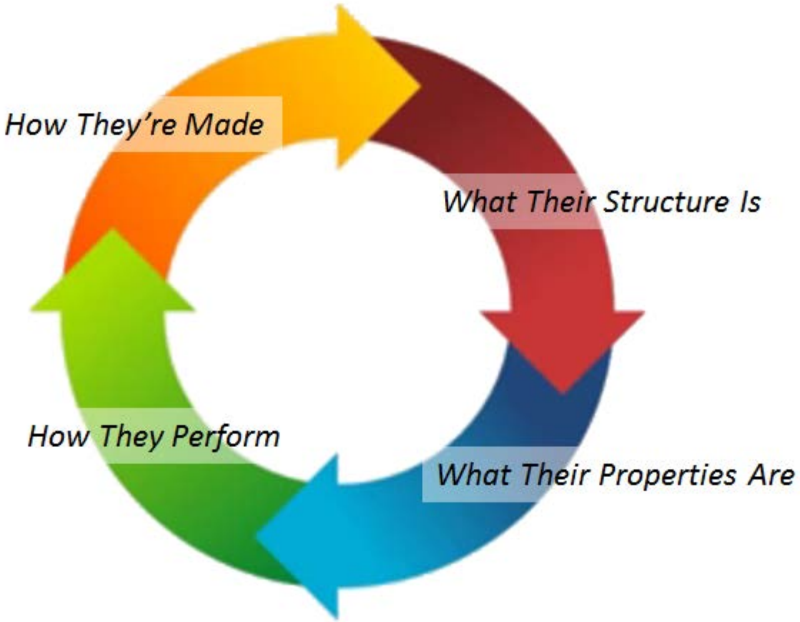


Beyond Kendall Square:

- Linking through ILP and Labs/Centers like MRL
- Embedding staff at MIT through Labs/Centers like MRL
- Collaborate in research

New Methods and Methodologies

Advances in imaging-based materials research:
Integrated in-situ studies of processing, structure, and properties
- Unprecedented nano/pico-scale structural and chemical analysis



Materials and process selection informed by system level assessment of

Integration of ab-initio simulations and machine learning in all aspects of materials research

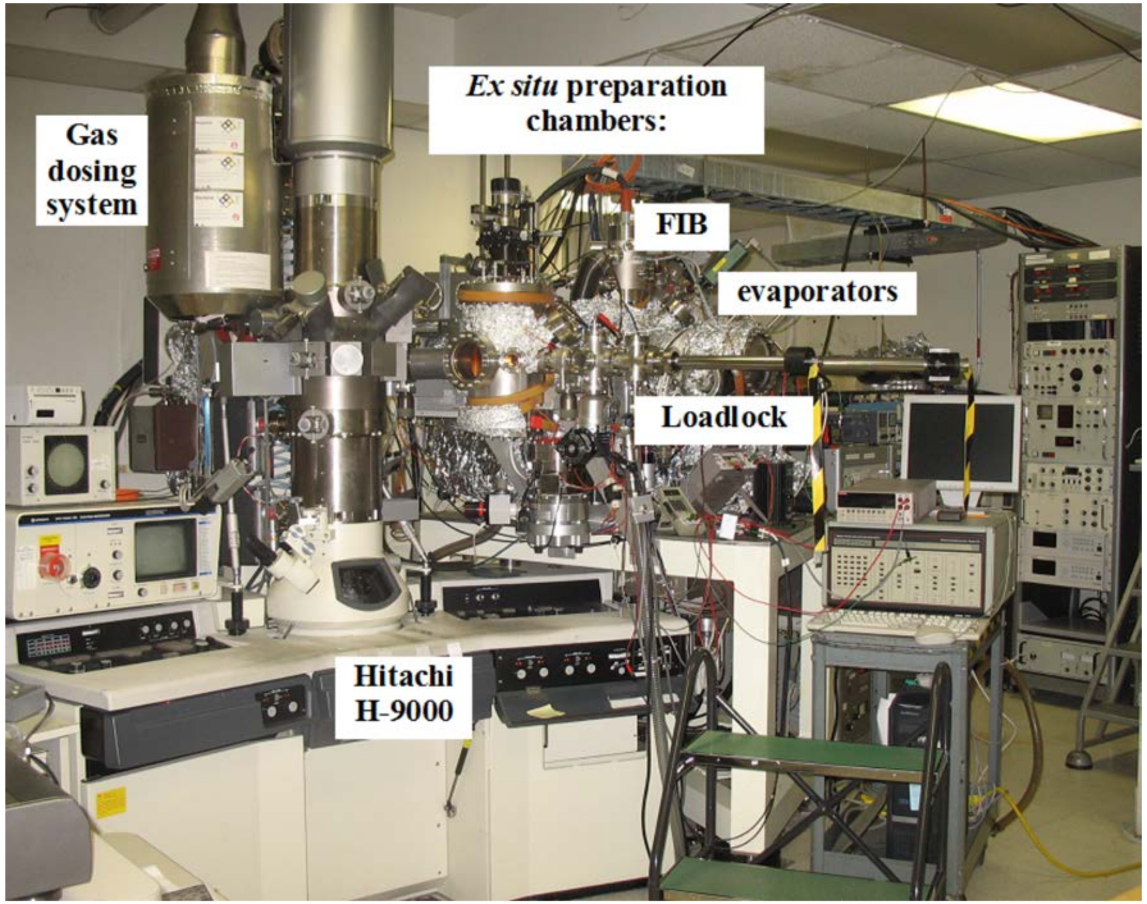
In situ Electron Microscopy for Materials and Process Design

Frances Ross, Department of Materials Science and Engineering (recently from IBM)

Heavily modified TEM for

- Ultra high vacuum/high resolution imaging
- Real-time imaging of gas phase and liquid phase materials synthesis

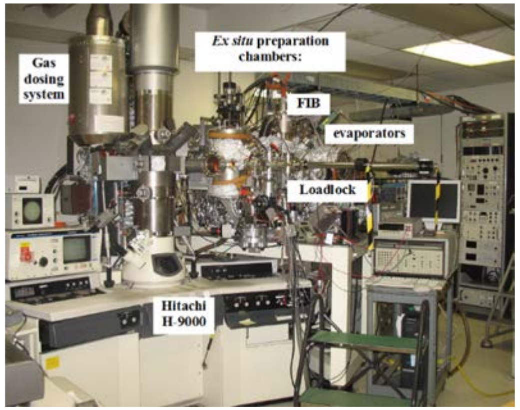
- Videos reveal atomic-level mechanisms of self assembly and growth of nanomaterials.
- This provides insights into process and materials design.

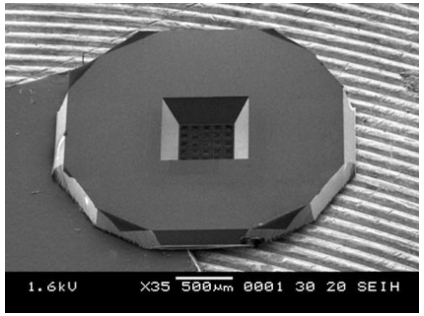


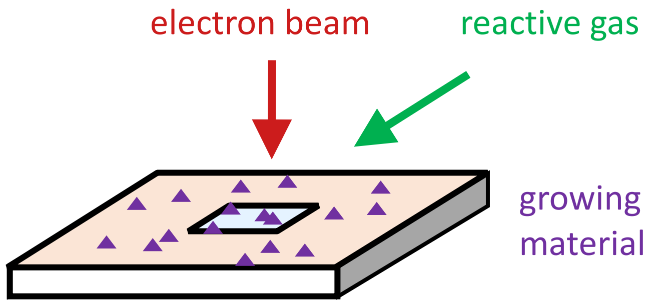
TEM for in situ studies to move from IBM to MRL.
Next generation microscope to be placed in MIT.nano

In-situ Imaging of Formation and Shape Evolution of Quantum Dots

Frances Ross, Department of Materials Science and Engineering (recently IBM)

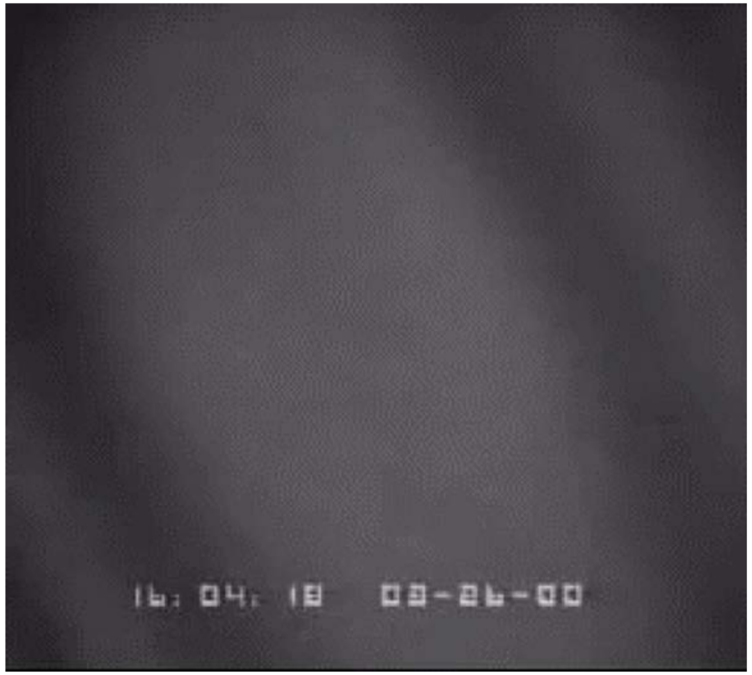




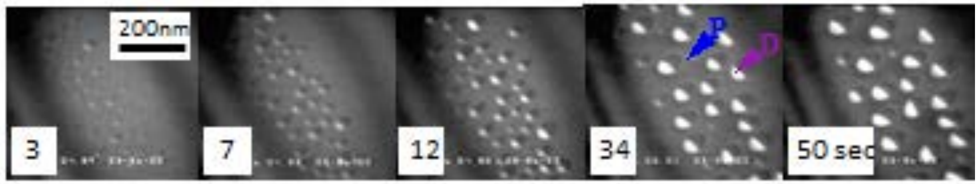


heated sample with central thin area for imaging

Introduce $GeSi_2$ to grow Ge quantum dots on heated Si substrate



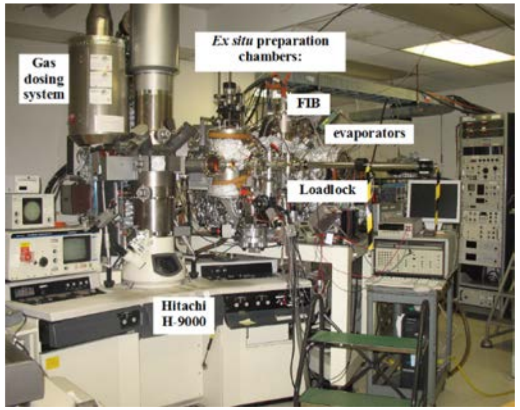
frame-by-frame analysis

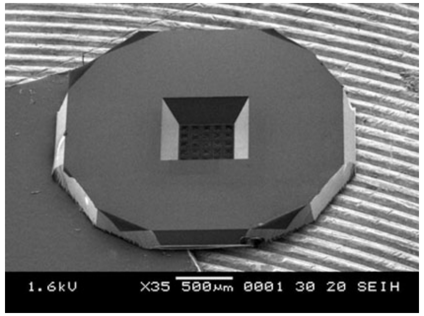


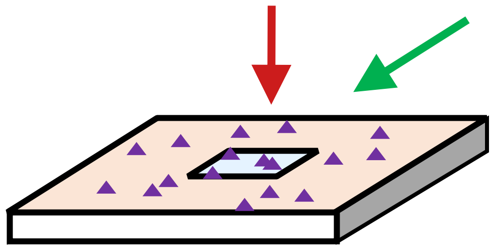
- Coarsening follows nucleation and growth
- Size dependent transition in facetted shape

In-situ Imaging of Formation and Shape Evolution of Quantum Dots

Frances Ross, Department of Materials Science and Engineering (recently IBM)







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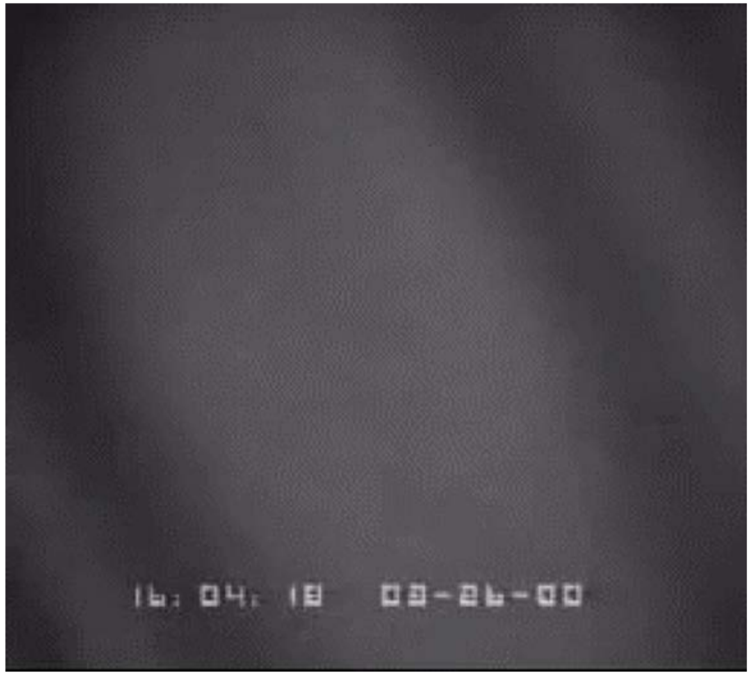
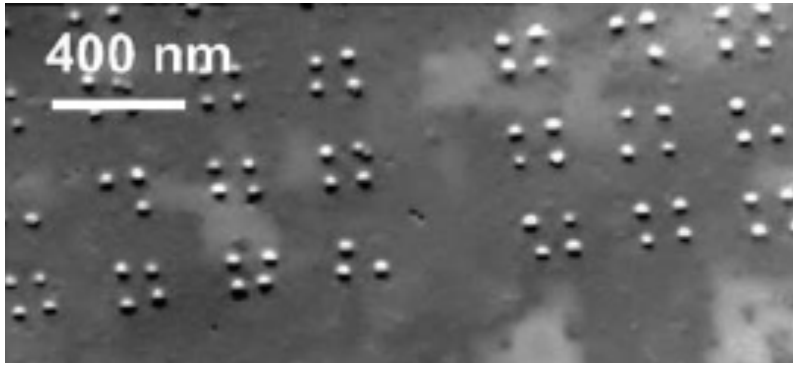


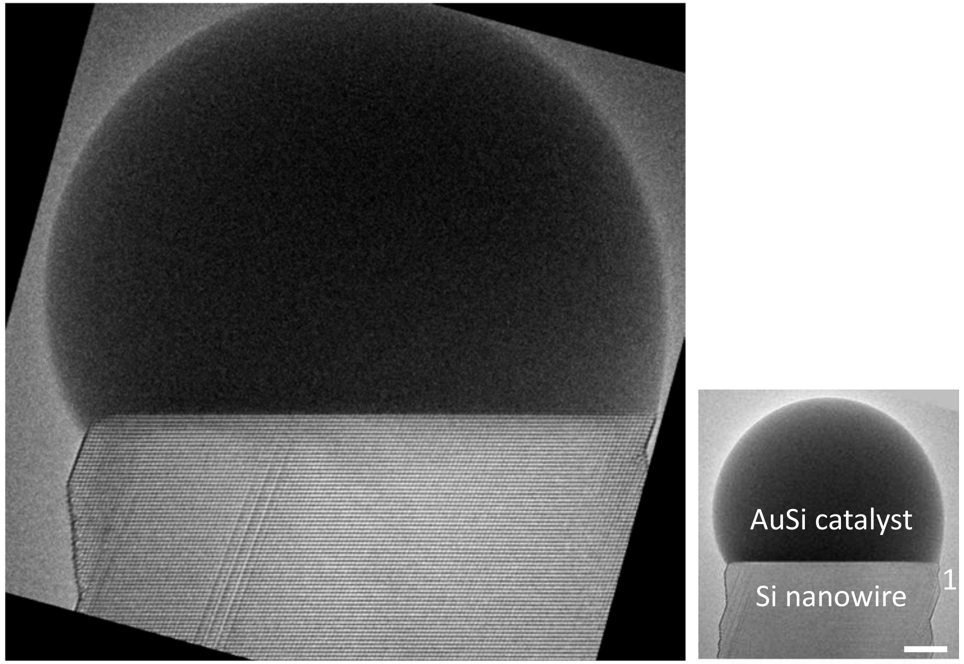
Control of nucleation and growth



In-situ Imaging of Growth of Nanowires

Frances Ross, Department of Materials Science and Engineering (recently IBM)

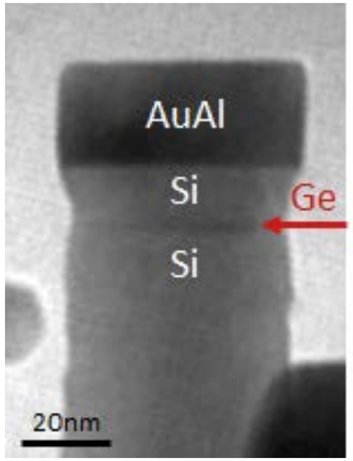
Nanowire growth through SiH_2 decomposition catalyzed by a liquid Au particle



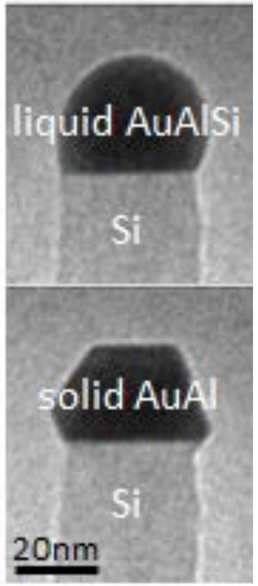
- Wire grows one atomic layer at a time
- Surface roughness due to nano-facets

Observing the details of this self-assembly process allows:

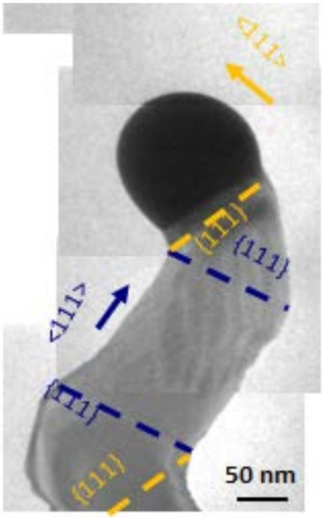
- Visualization of the atomic pathways
- Development of models for growth
- Generation strategies for precise control
- Identification and anticipation of new growth modes



Growth of a complex structure through catalyst design



Fundamentals of phase transformations

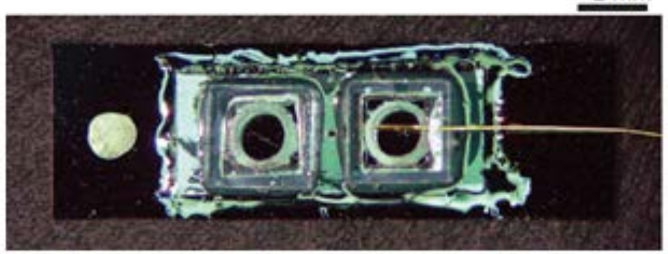


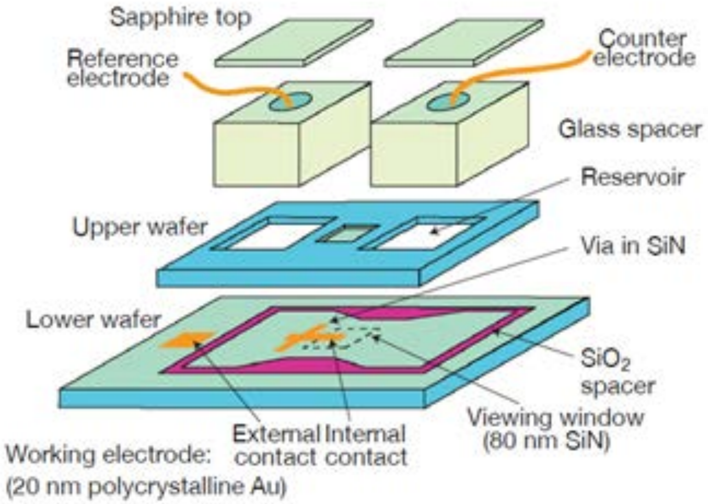
Control of growth direction using an electric field

In-situ Imaging Liquid Phase Processes

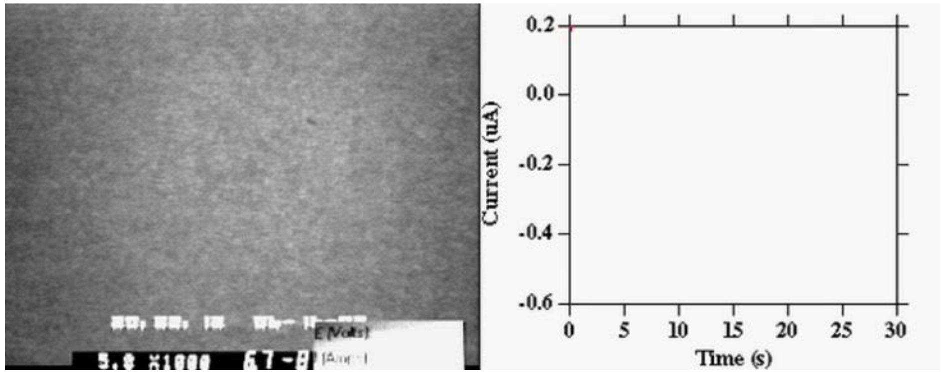
Frances Ross, Department of Materials Science and Engineering (recently IBM)

First to Design, Build and Use Liquid Cells for in situ TEM

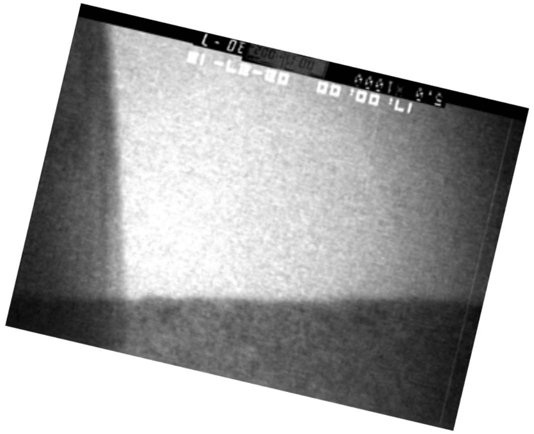




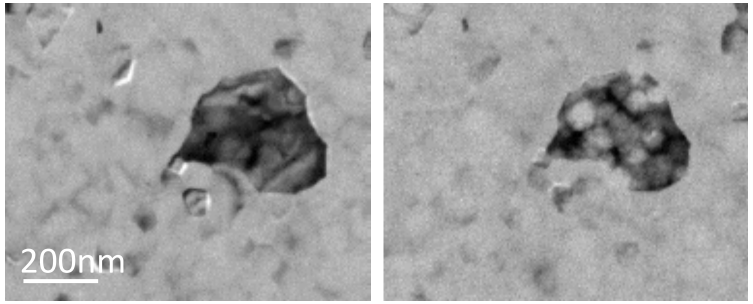
In-situ observation of Cu electrodepostion



In situ observation of the onset of dendritic growth during electrodeposition



In situ observation of intragranular pitting during corrosion of Al



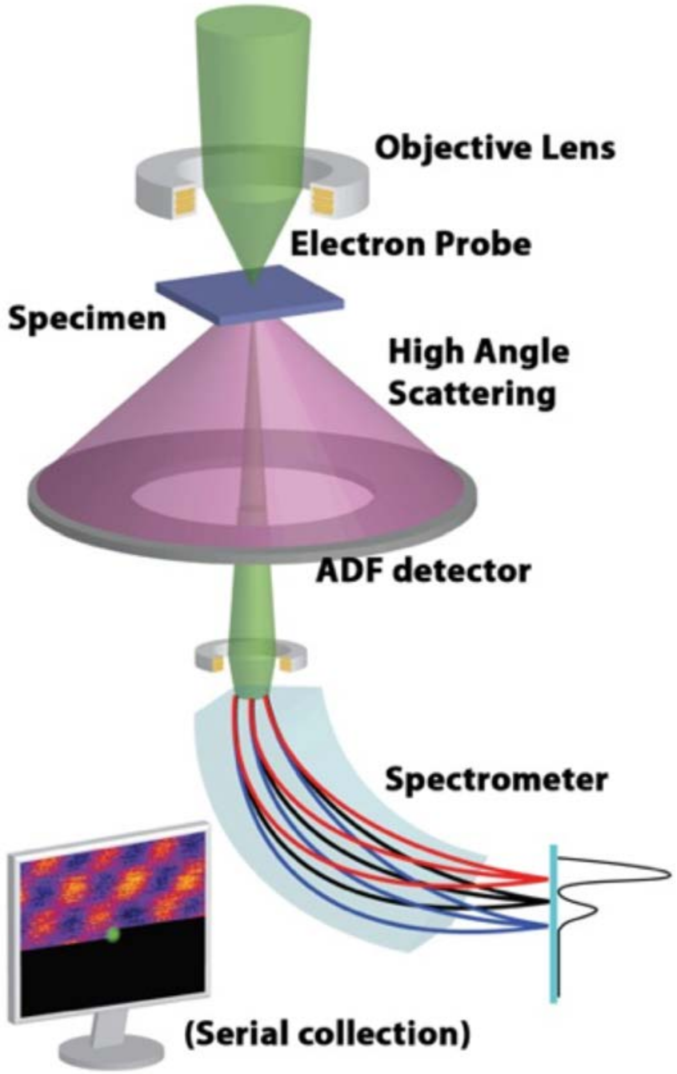
Advancing the State-of-the-Art Transmission Electron Microscopy: Pico-scale Imaging

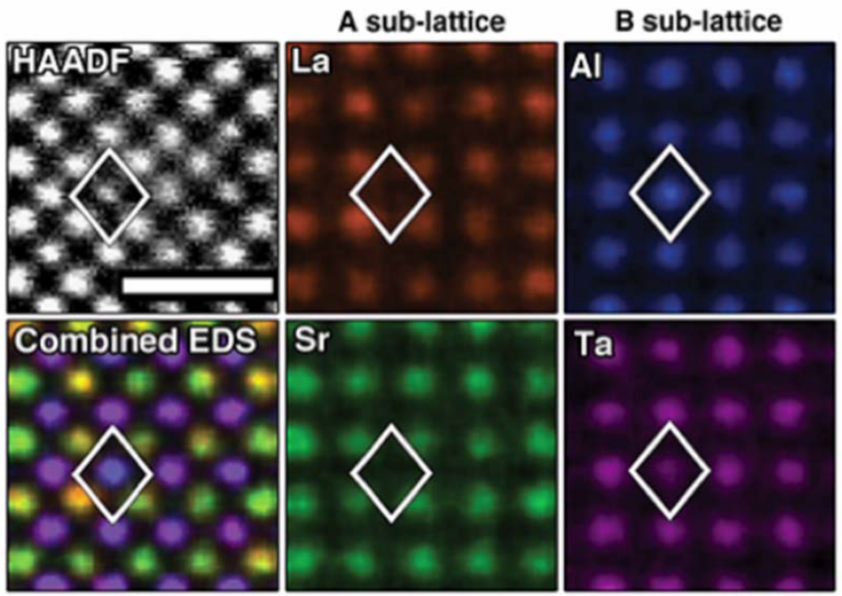
Jim LeBeau, Department of Materials Science and Engineering, Spring 2019

- Key to the materials feedback loop: synthesize, characterize, properties

- Requires extreme environmental stability (vibrations, fields, temperature)

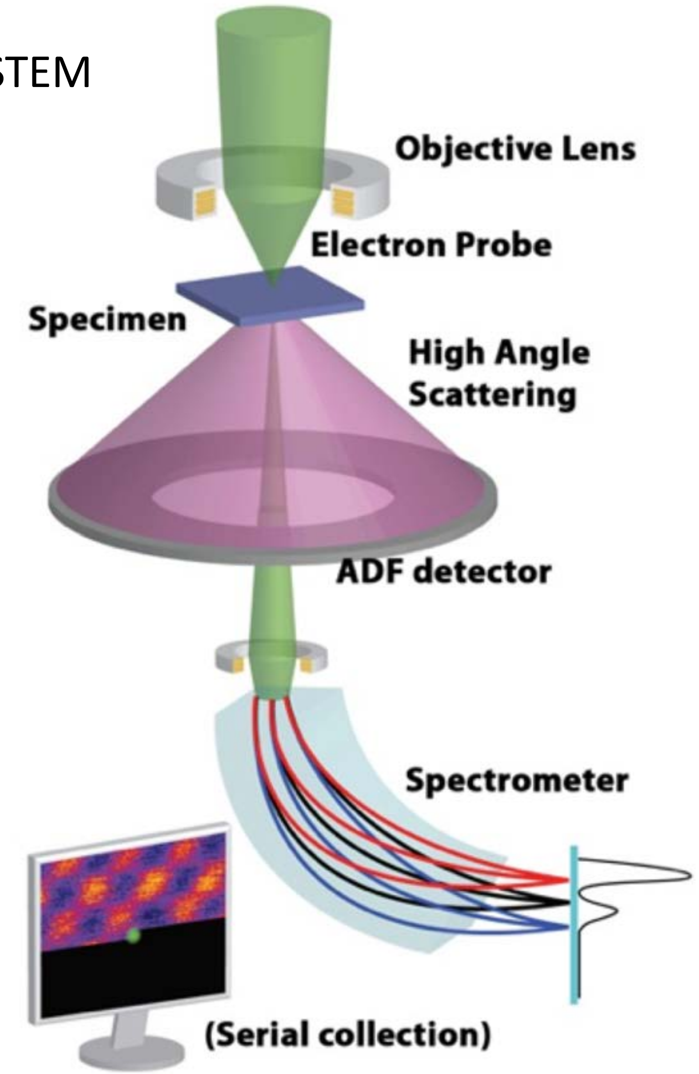
- ***Picometer*** deflections of inelastically scattered electrons provide **sub-atomic resolution**. Electron energy loss spectroscopy provides **atom identity.**



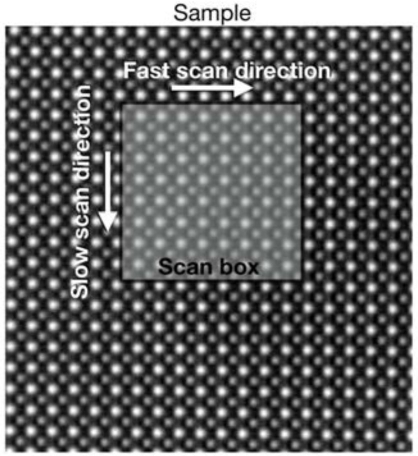


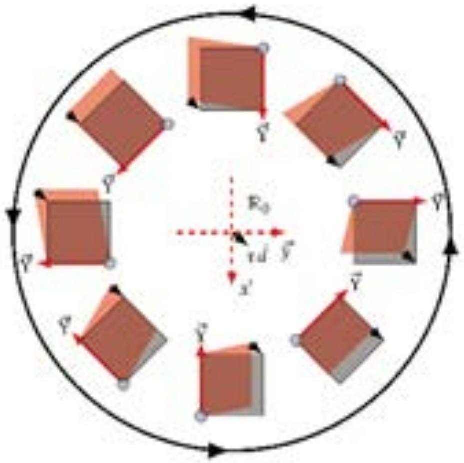
Advancing the State-of-the-Art Transmission Electron Microscopy: Pico-scale Imaging

STEM



RevSTEM: Correction for Sample Drift

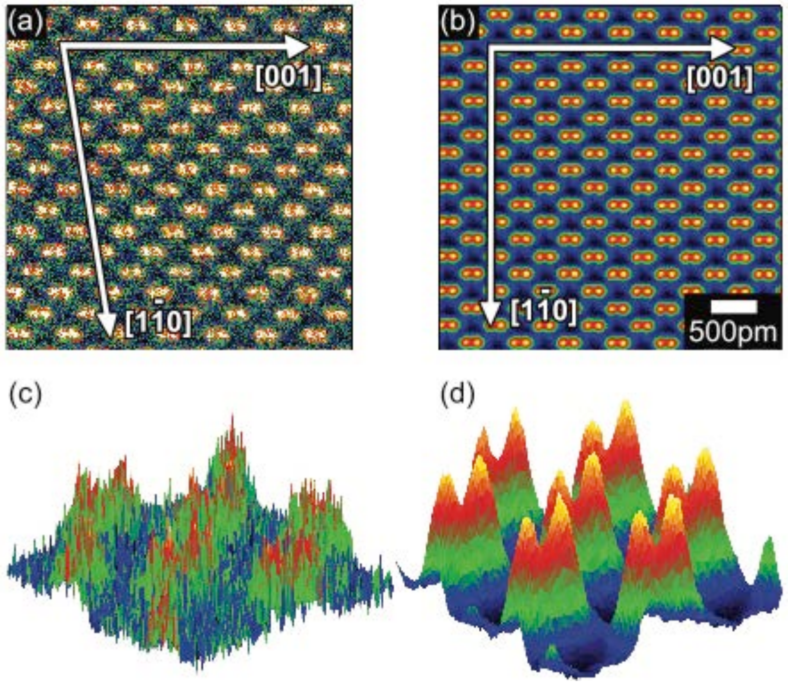




collect images in 4 or 8 locations

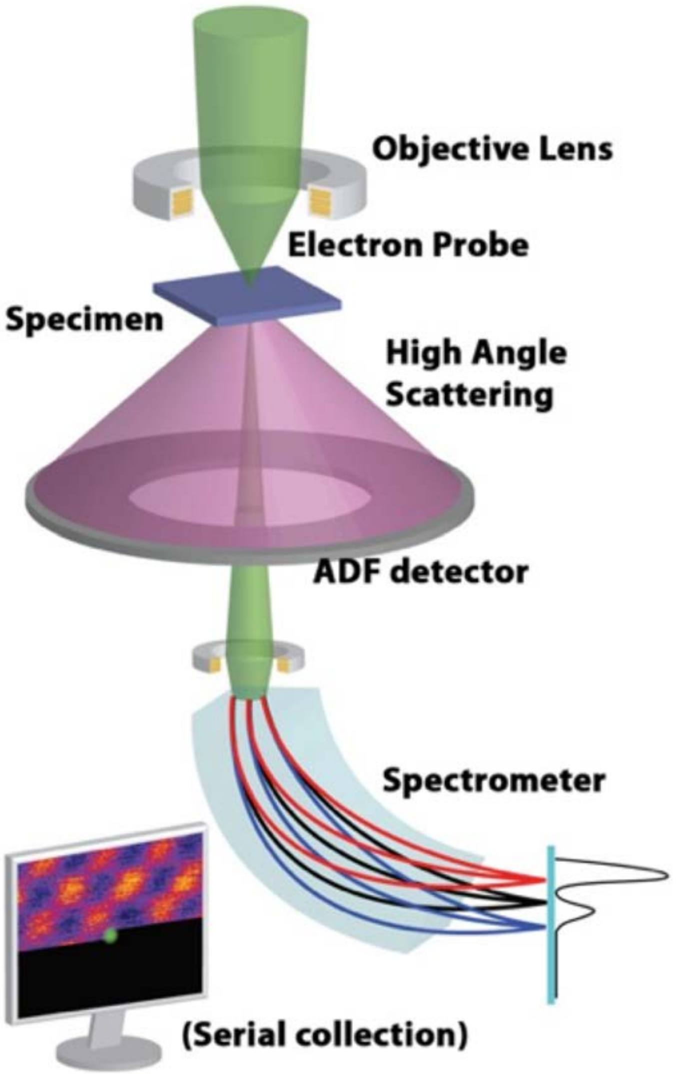
w/o RevSTEM

w/RevSTEM

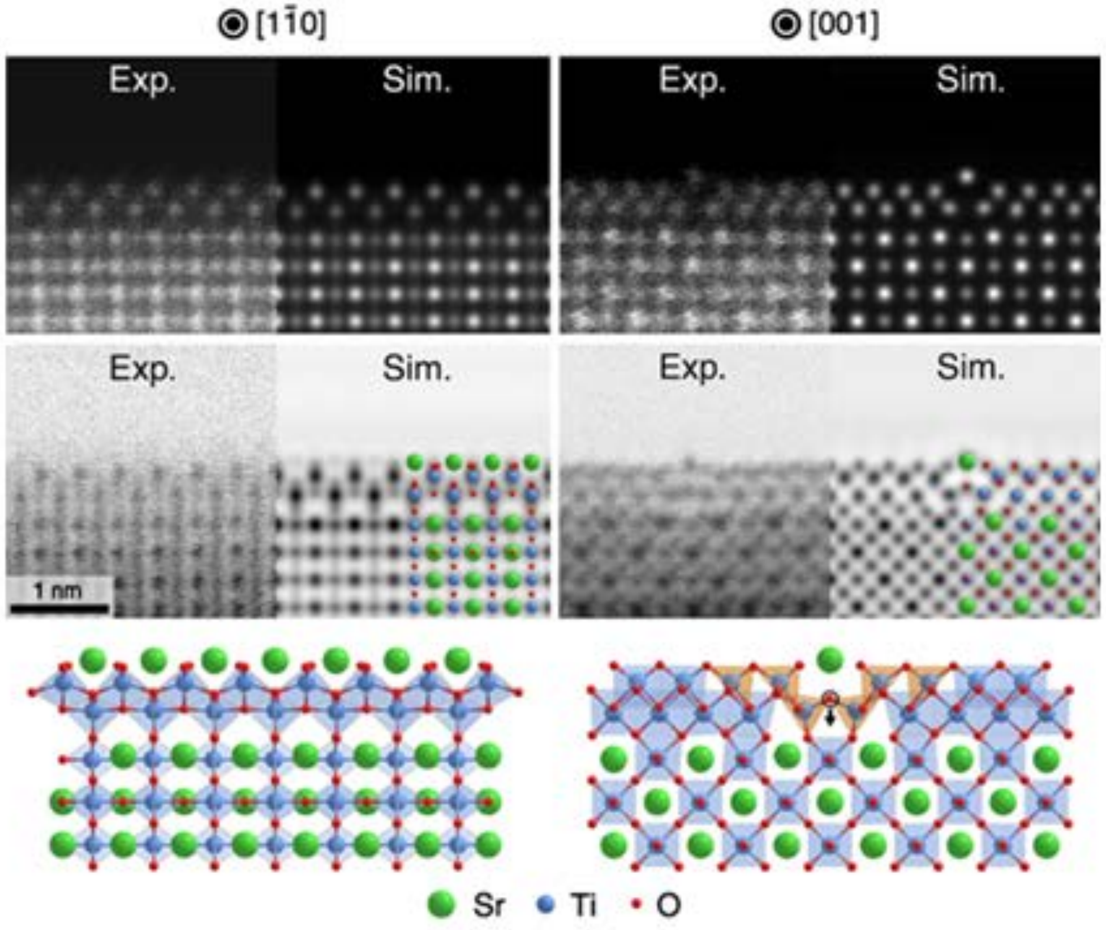


10^3 improvement in accuracy

Advancing the State-of-the-Art Electron Microscopy: Pico-scale Imaging



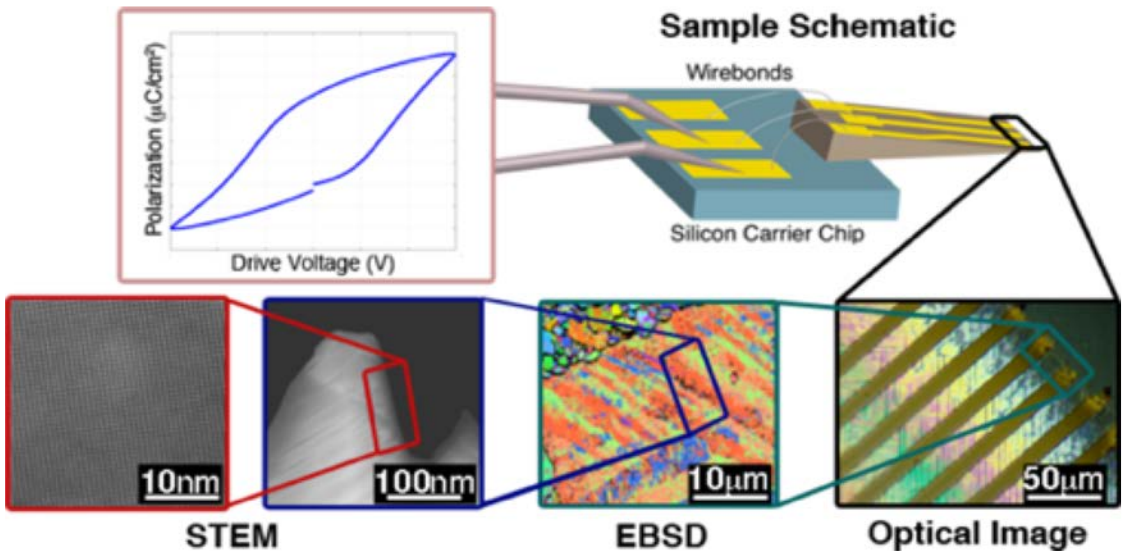
Atomic/chemical resolution at surfaces: Surface Reconstruction

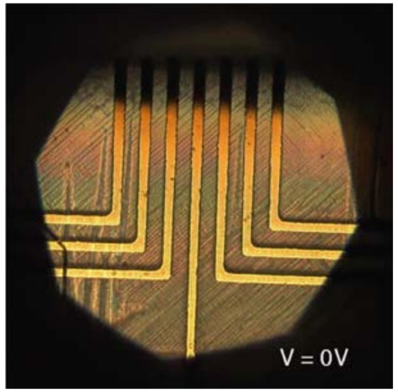


quantum mechanical simulations play a key role

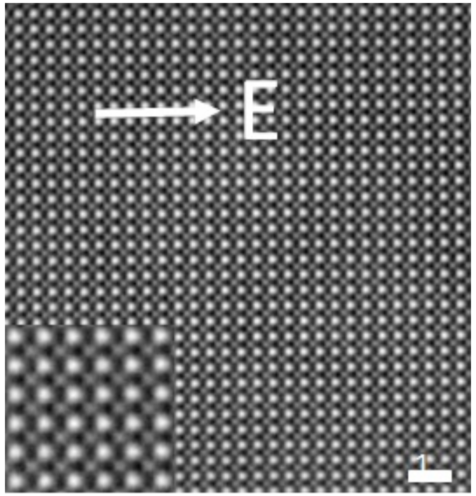
In situ Fields – From Macroscale to Atomic Scale

A multiscale biasing platform

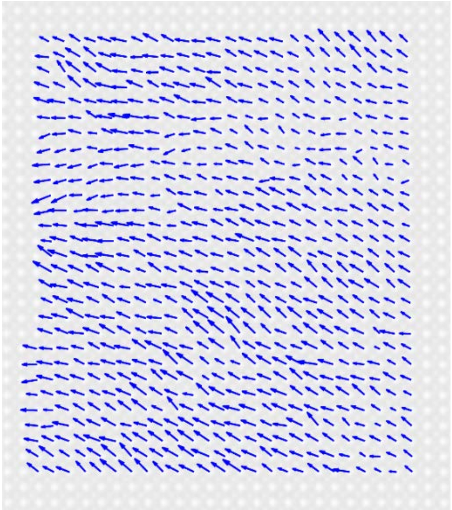




Applied Field

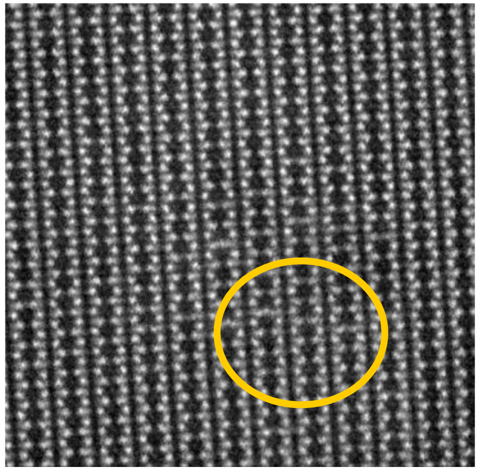


Cation Shifts



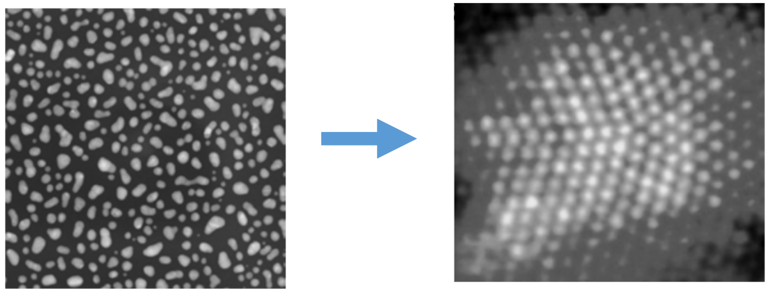
Future direction

Point defect migration

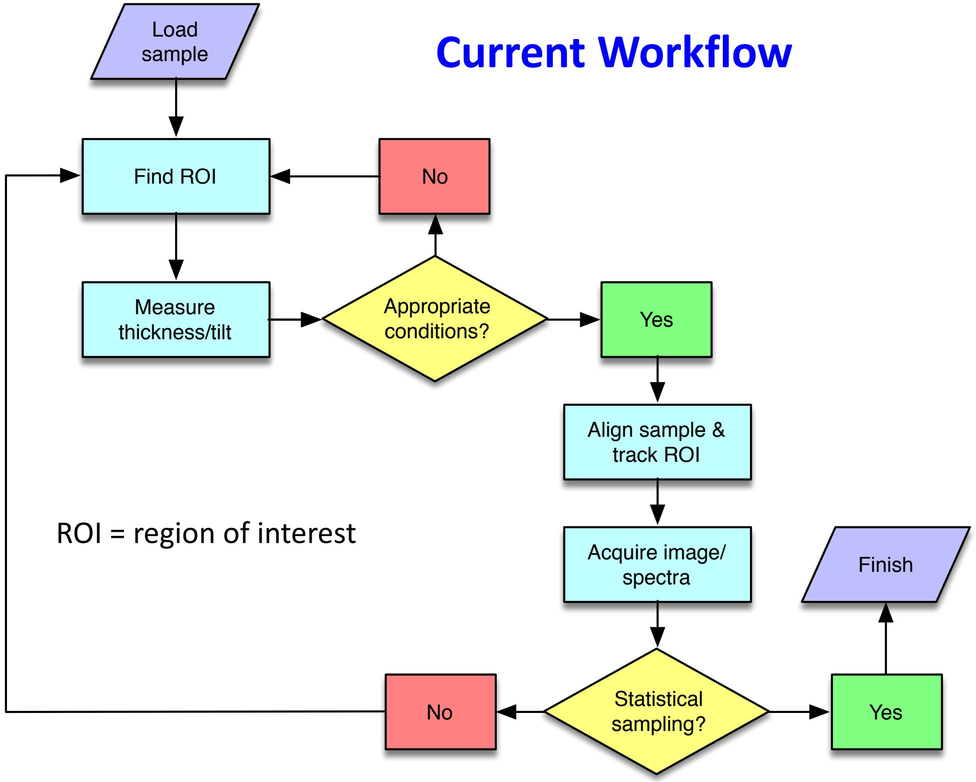


Machine Learning For Atomic Resolution Electron Microscopy

e.g. Atomic Imaging of Nanoparticles

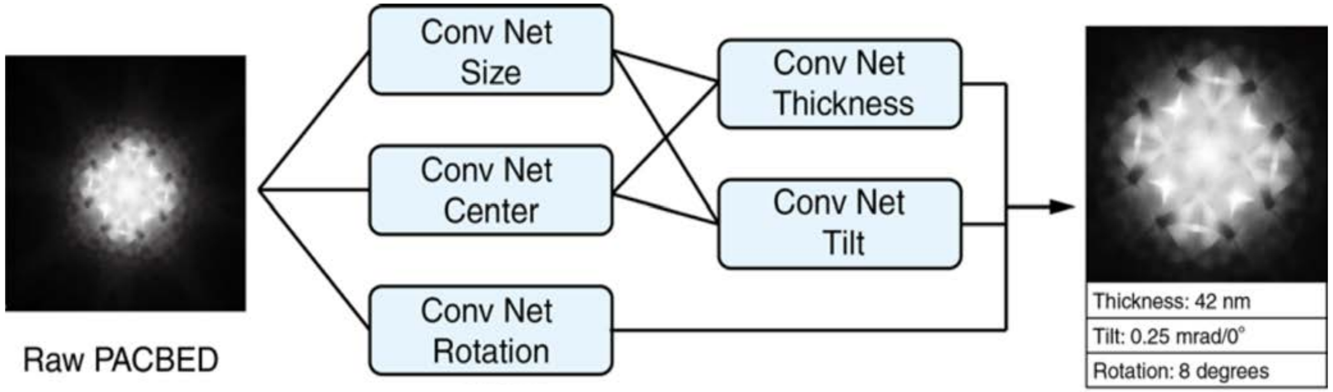


Current Workflow



ROI = region of interest

Convolutional Neural Network for Autonomous Diffraction Analysis



Find thickness, tilt and rotation from a single Position Averaged Convergent Beam Electron Diffraction pattern

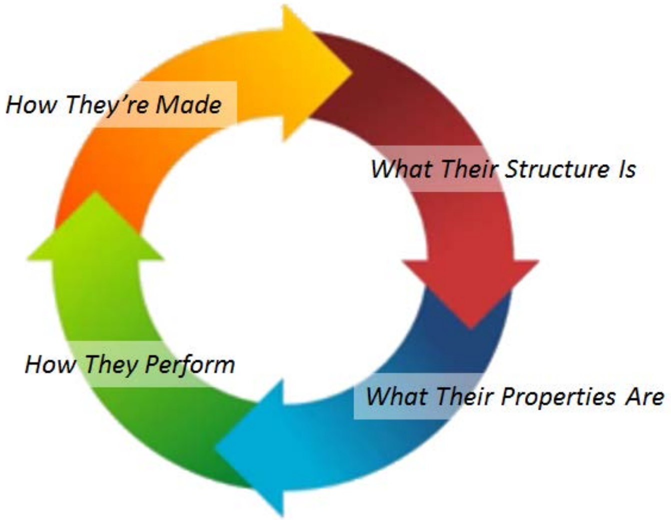
Train neural network using quantum mechanical simulation of images

Next steps: Instrument feedback control, robust ROI tracking, autofocus, auto acquire

The Quality of the Imaging Space in MIT.nano and Embedding in the MIT Environment Will Support a New Wave of Innovation in Imaging-Based Materials Research

New Methods and Methodologies

Advances in imaging-based materials research:
Integrated in-situ studies of processing, structure, and properties
- Unprecedented nano/pico-scale structural and chemical analysis



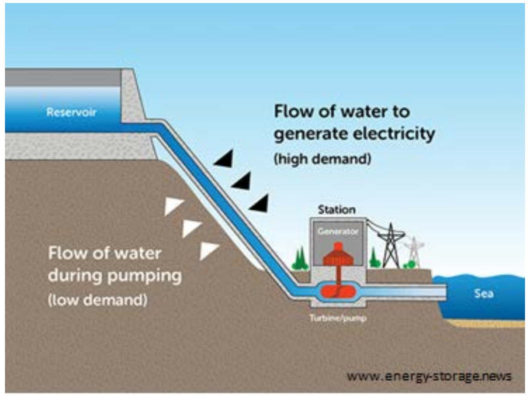
Materials and process selection informed by system level assessment of
- Performance
- Cost over the full life-cycle of the material
- Abundance
- Environmental and Societal Impact

Integration of ab-initio simulations and machine learning in all aspects of materials research

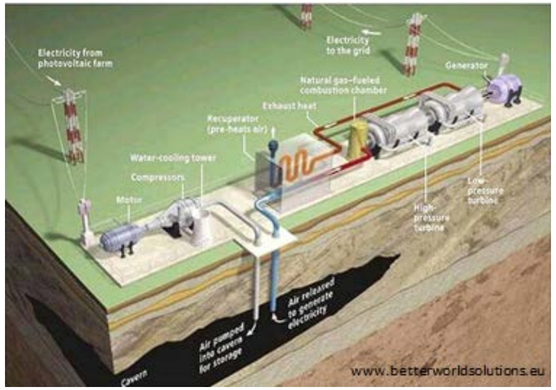
Determining What Materials and Systems to Target for Research

Renewable Energy Sources are Intermittent

Energy Storage to Match Demand and Reduce Cost



pumped hydro storage



compressed air storage

What is Required for Batteries to Lower Costs

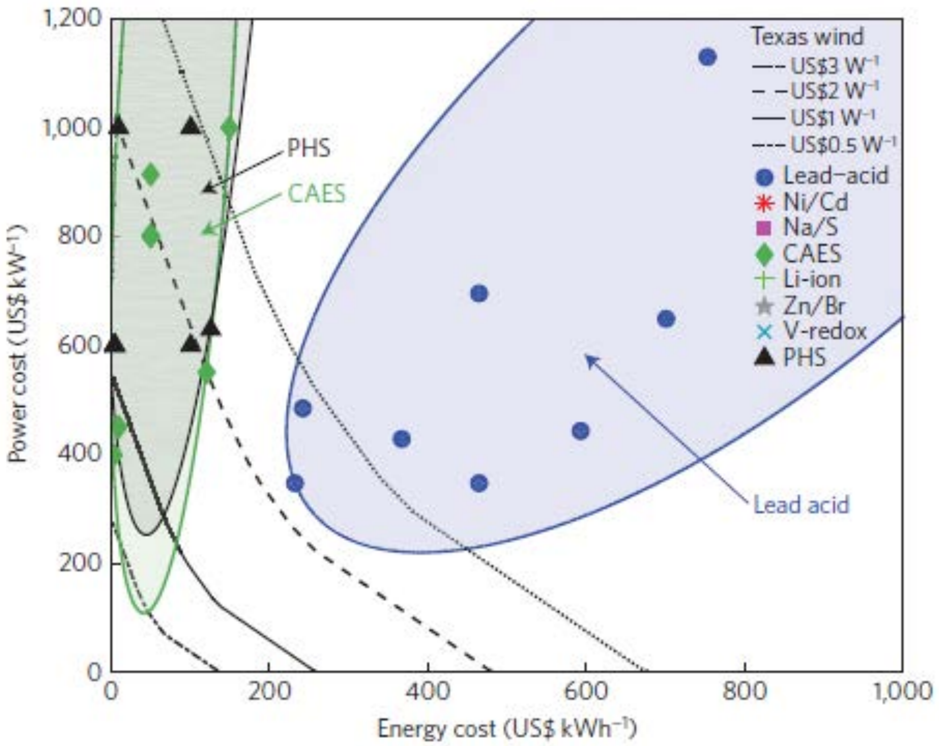
It depends on

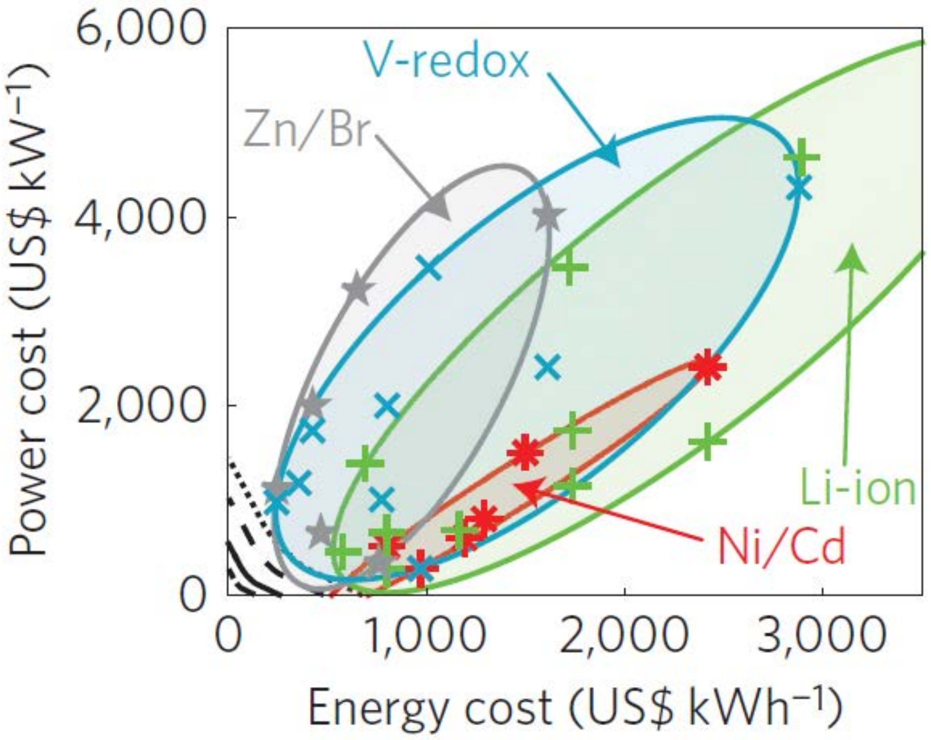
- energy source
- location
- type of battery

When do Batteries Reduce Costs for Renewable Energy Sources

Jessika Trancik: Institute for Data, Systems, and Society

CAES: compressed air energy storage; PHS: pumped hydro storage; lead–acid, Ni/Cd, Na/S, Li-ion: batteries; Zn/Br, V-redox: flow batteries.



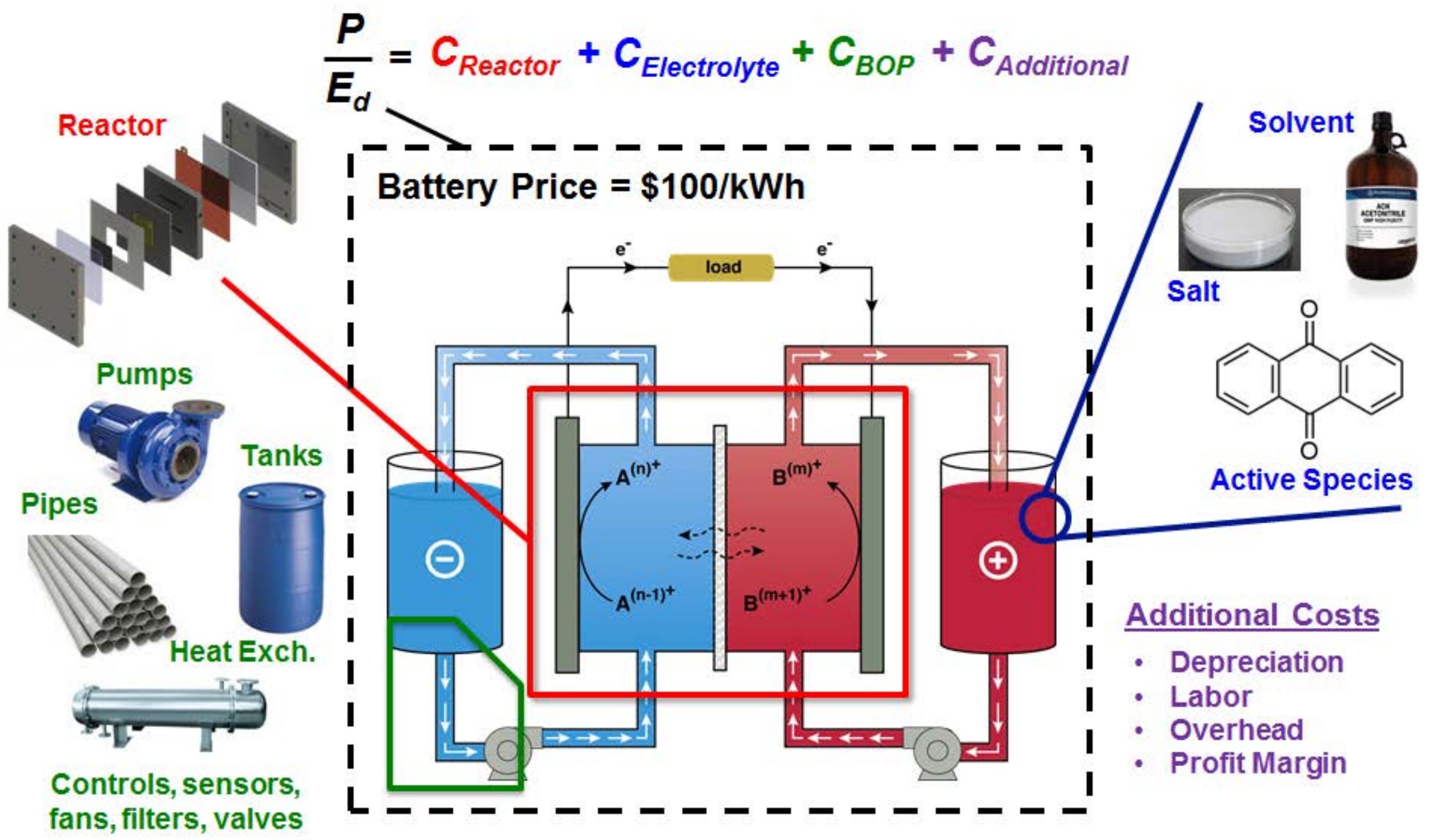


lines: threshold storage cost intensities at which it becomes valuable to incorporate storage

Output: Cost targets

Techno-Economic Analysis to Identify Key Challenges and Performance Needs in Electrochemical Energy Storage: Redox Flow Batteries

Fikile Brushett: Chemical Engineering

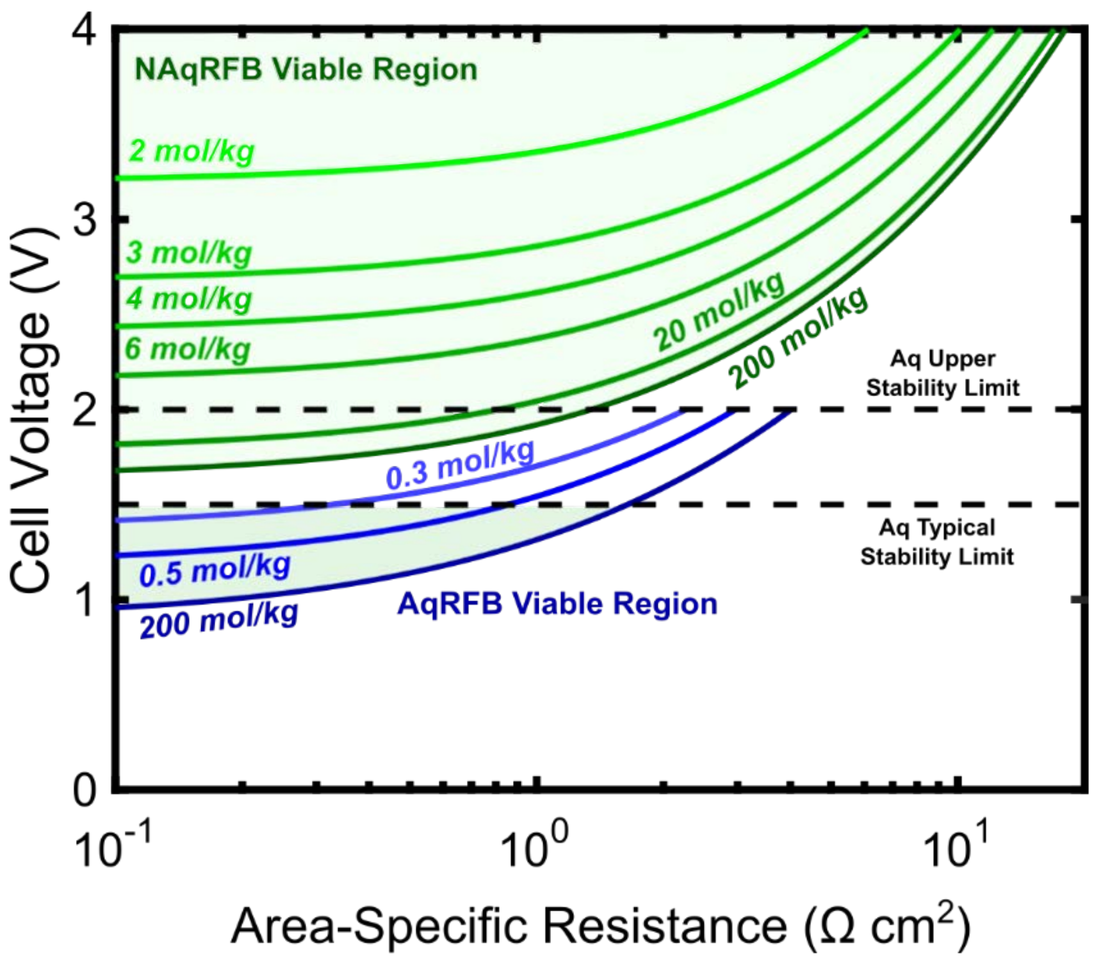


Connecting system-level performance and cost goals to materials-level property requirements to guide the development of the new chemistries and reactor designs

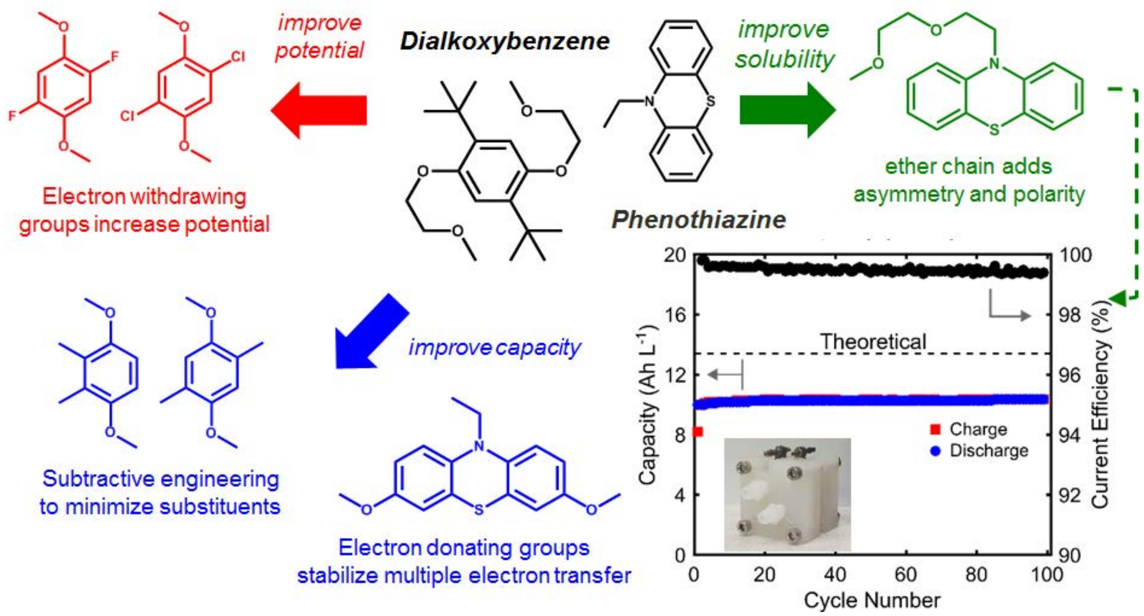
Speaker today

Techno-Economic Analysis to Identify Key Challenges and Performance Needs in Electrochemical Energy Storage: Redox Flow Batteries

Fikile Brushett, Chemical Engineering



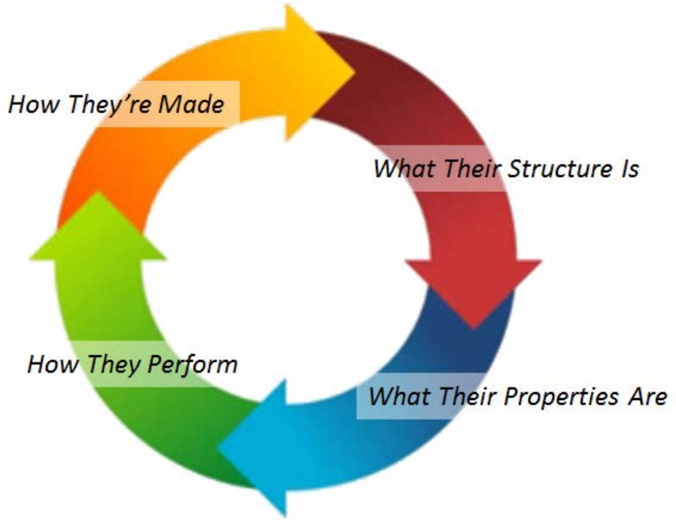
Cost analysis drives research on reactor materials and active species



Connecting system-level performance and cost goals to materials-level property requirements to guide the development of the new chemistries and reactor designs

New Methods and Methodologies

Advances in imaging-based materials research:
Integrated in-situ studies of processing, structure, and properties
- Unprecedented nano/pico-scale structural and chemical analysis



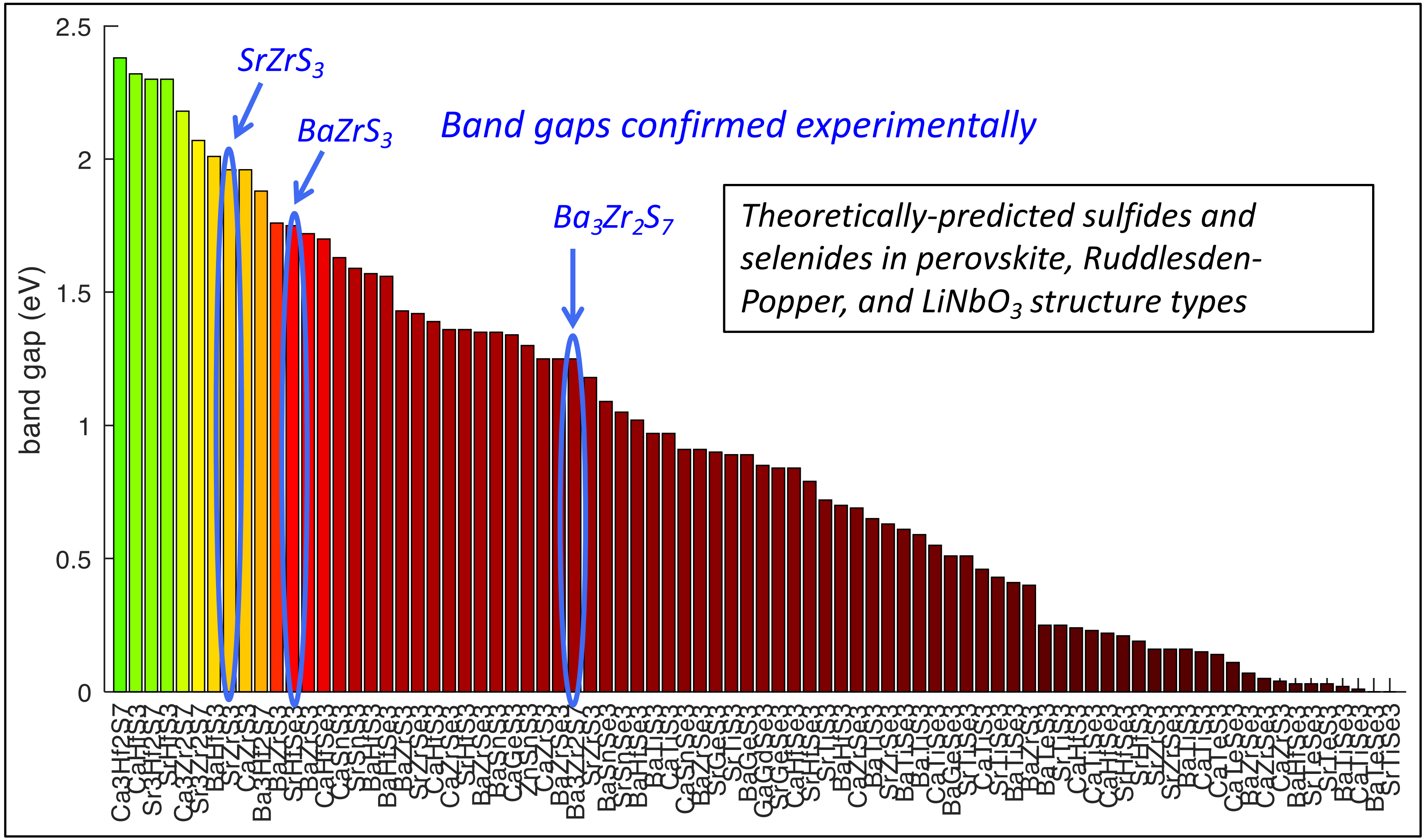
Materials and process selection informed by system level assessment of
- Performance
- Cost over the full life-cycle of the material
- Abundance
- Environmental and Societal Impact

Integration of ab-initio simulations and machine learning in all aspects of materials research

Chalcogenide Active Materials for Photonics and Photovoltaics

Rafael Jaramillo, Department of Materials Science and Engineering

Before: experiments → theory Today: theory → experiment

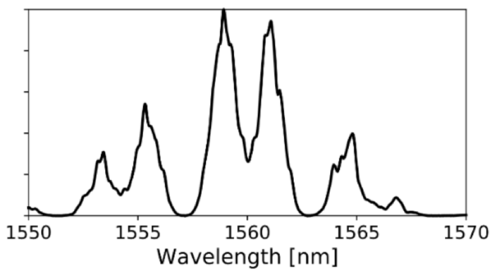


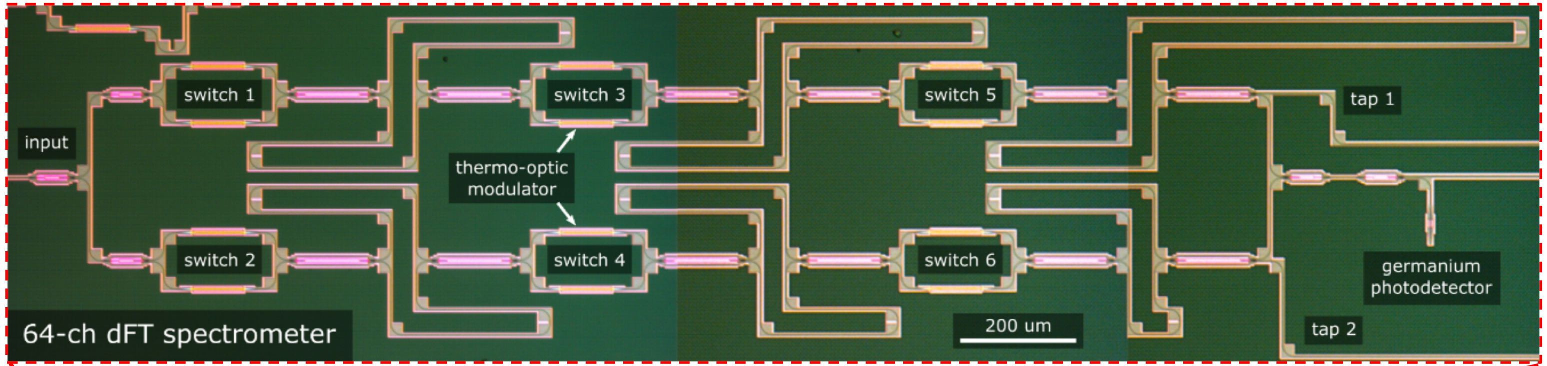
Speaker today

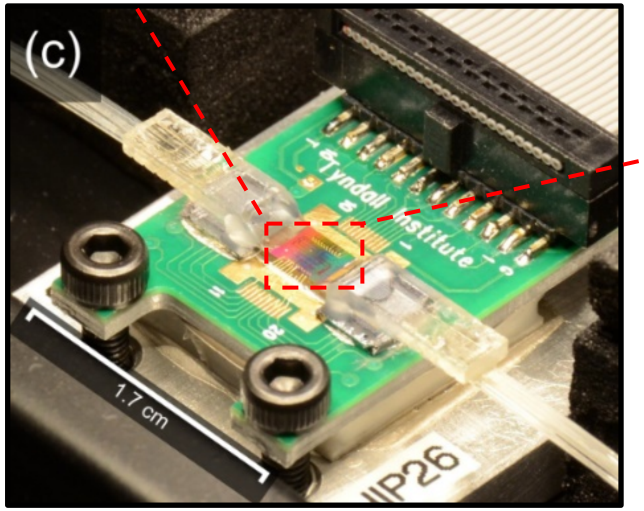
Machine-learning-enhanced Chip-scale Spectrometers for Chemical Sensing

Juejen (JJ) Hu, Department of Materials Science and Engineering
Brando Miranda, Center for Brains Minds and Machines, MIT

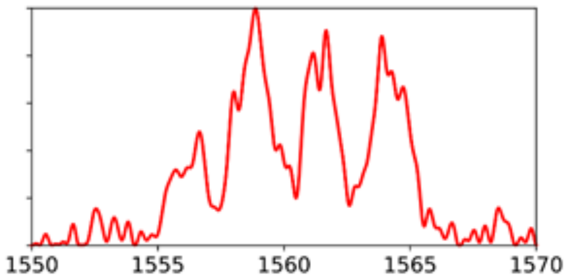
spectrum in







intensity out



- measure intensity of light out for 64 states
- determine the spectrum using machine learning
- performance improves exponentially with the number of switches

Speaker today

Vision for Computer Aided, Data-driven Materials Discovery

Move from this:

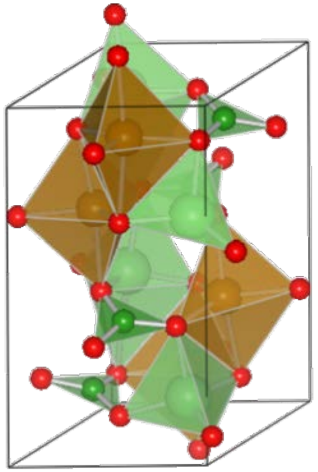
1. Identify material to make
2. Read literature/do what you did last time
3. Trial-and-error synthesis

…to this:

1. A computer helps you decide what to make
2. And suggests how to make it
3. Synthesize material

The Materials Genome/Project: Modern data-driven and first-principles materials design accelerates pace for knowing *what* to make…

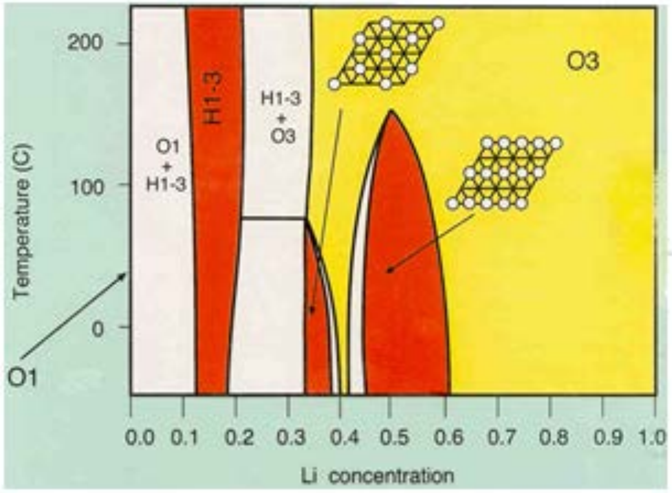
Data Mining of Compilations of Known Structures



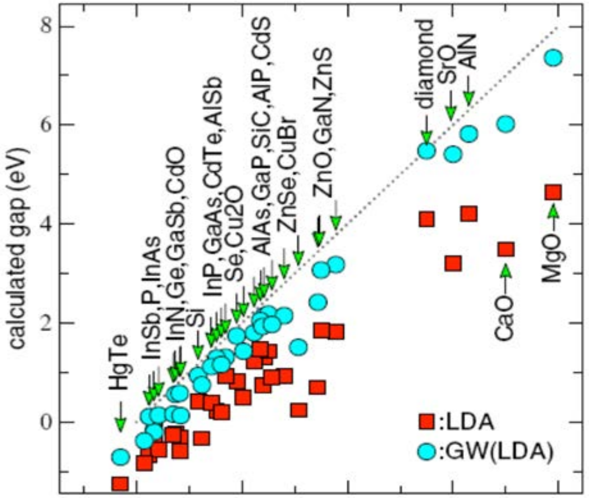
+

First Principles Calculations
- Thermodynamic Stability
- Properties

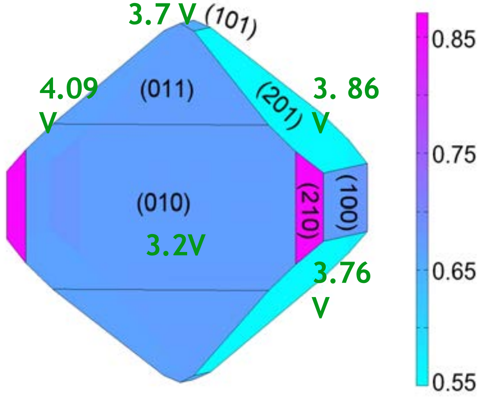
$$H = \sum_{i=1}^{N_e} \nabla_i^2 + \sum_{i=1}^{N_e} V_{nuclear}(r_i) + \frac{1}{2}\sum_{i}^{N_e}\sum_{j\neq i}^{N_e}\frac{1}{|r_j - r_i|}$$



Phase diagrams



Bandgaps

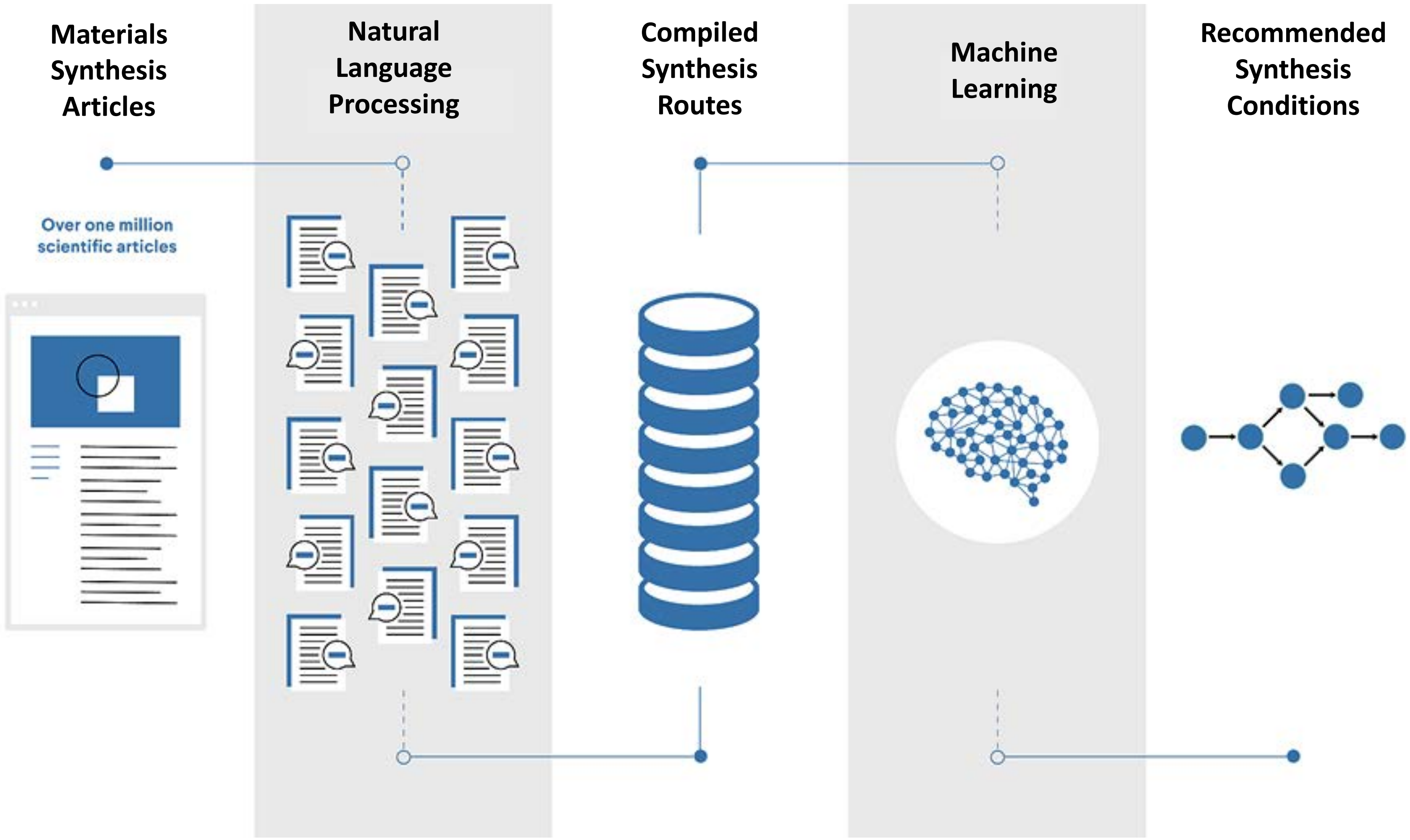


Surfaces

Elsa Olivetti with attribution to G. Ceder

Virtual Screening for Inorganic Materials Synthesis Parameters Using Deep Learning Methods

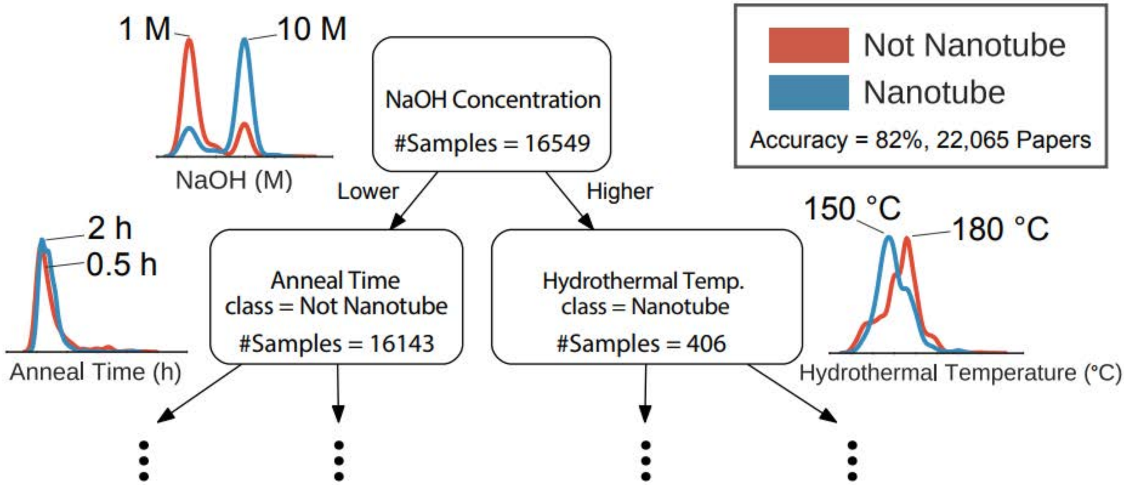
Elsa Olivetti, Department of Materials Science and Engineering



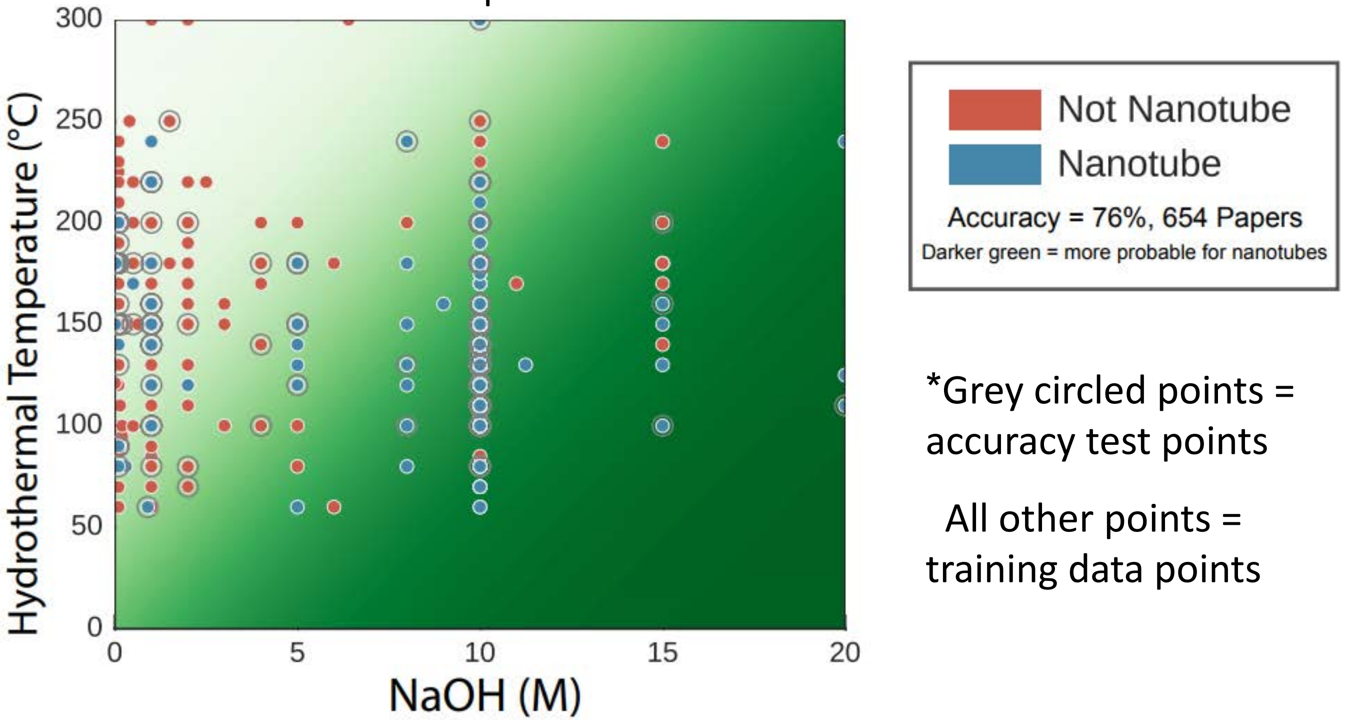
Example: Suggesting Synthesis Conditions for a Specific Morphology of Titania (TiO_2)

Elsa Olivettti, Department of Materials Science and Engineering

22,065 papers



Of 27 process variables, the two most important



*Grey circled points = accuracy test points

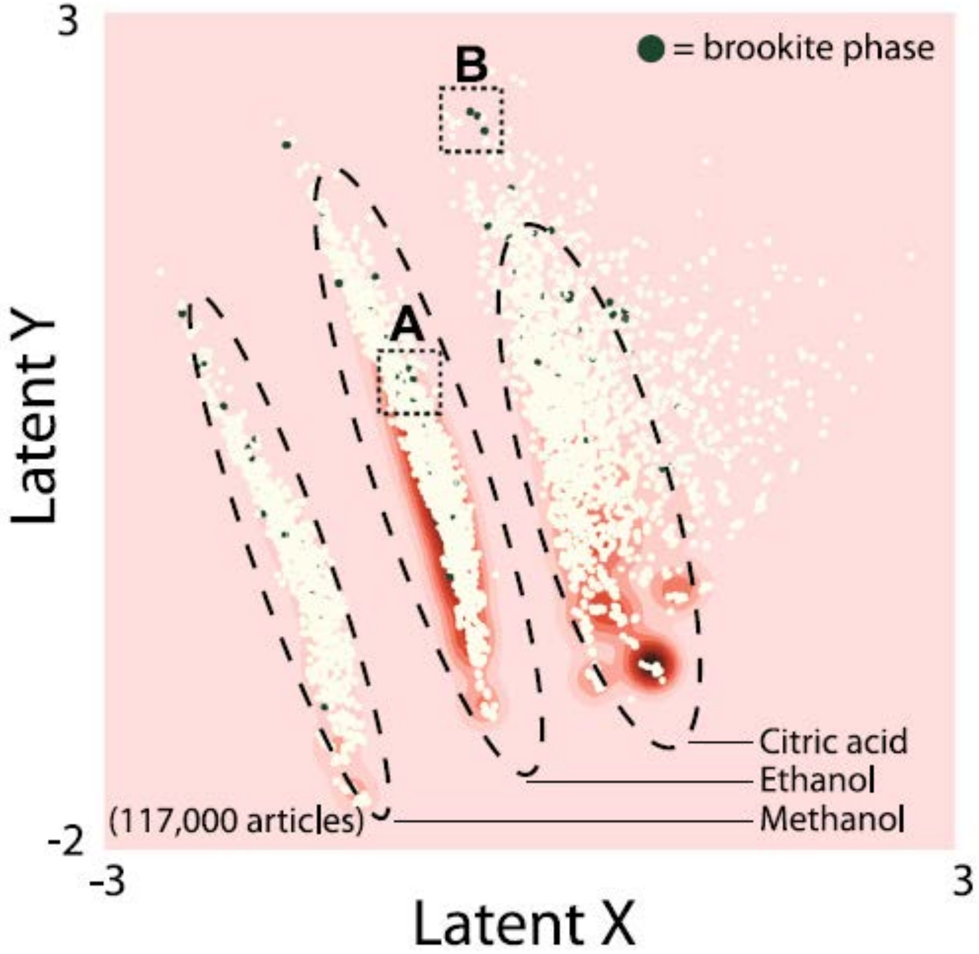
All other points = training data points

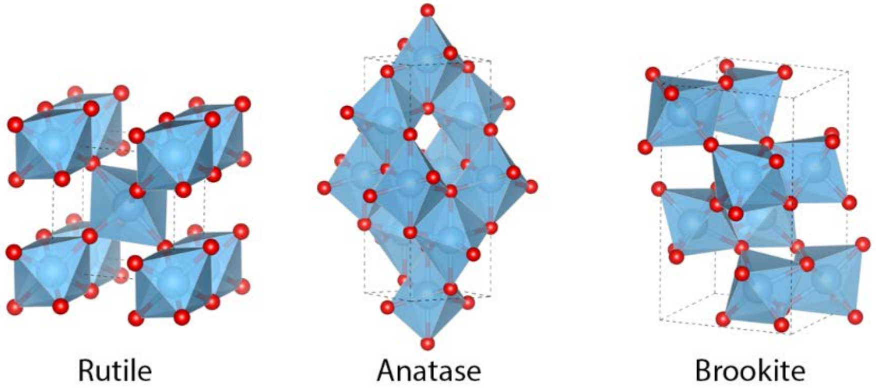
Experimentally-accessible (and reported) variables to facilitate practical synthesis route planning.

Edward Kim et al., *Chemistry of Materials 2017*

Exploratory: Rare Phase in Common Material

Elsa Olivettti, Department of Materials Science and Engineering
Stefanie Jegelka, Computer Science and Artificial Intelligence Laboratory, EECS



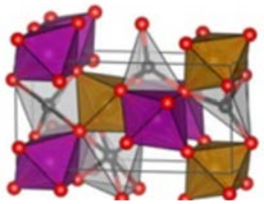


Clustering of latent space shows driving conditions for polymorph of TiO_2 for photocatalysis

E. Kim et al., npj Computational Materials 2017

Example: Suggesting Synthesis Conditions for Stabilizing Desired Materials Structures

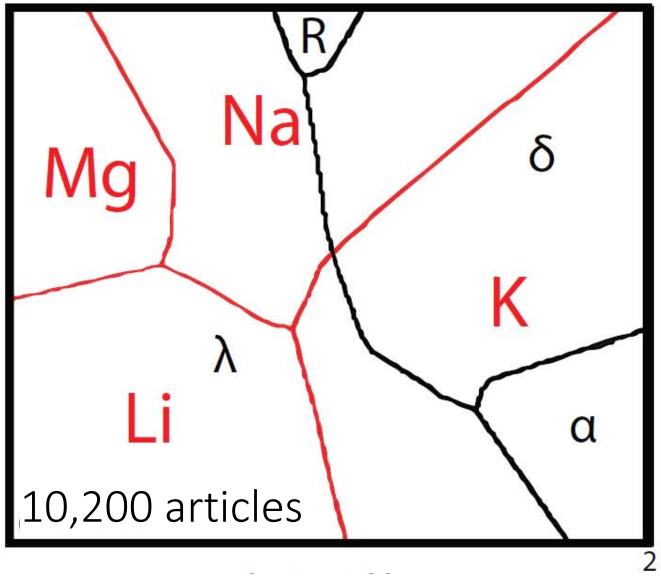
Elsa Olivettti, Department of Materials Science and Engineering
Stefanie Jegelka, Computer Science and Artificial Intelligence Laboratory, EECS

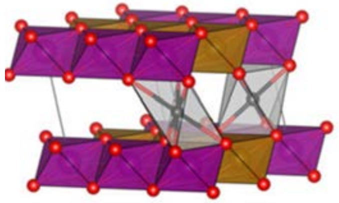

Ramsdellite (R)

Alkaline batteries

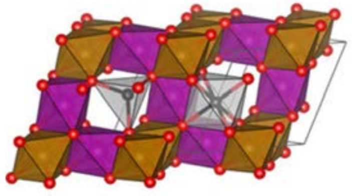
Photocatalysts

Polymorphs for MnO_2 overlaid with most probable alkali-ion use in synthesis (intercalation-based phase stability)

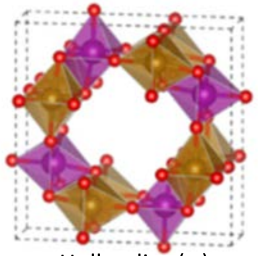



Birnessite (δ)

Lithium-ion batteries


Spinel (λ)

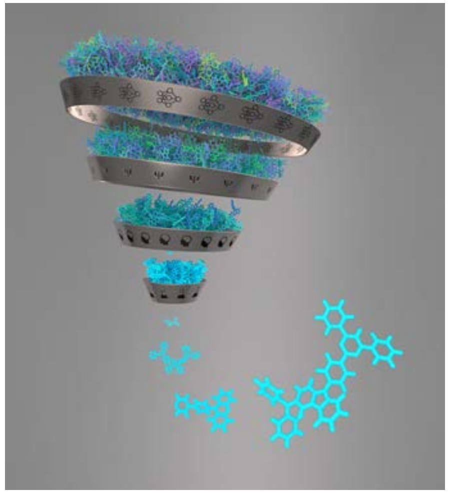
Molecular sieves

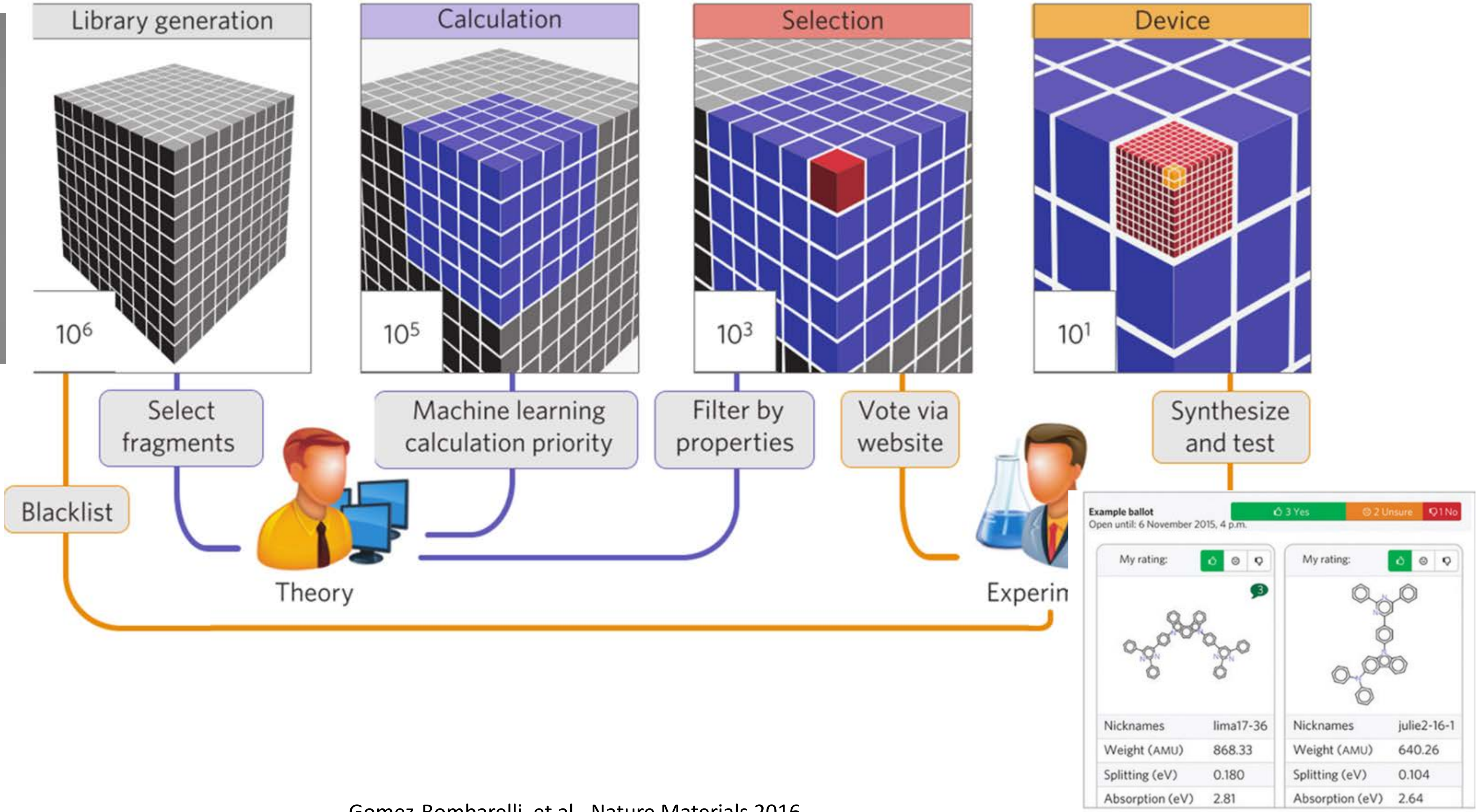

Hollandite (α)

E. Kim et al., npj Computational Materials 2017

High-Throughput Virtual Organic Molecule Screening

Rafael Gomez-Bombarelli, Department of Materials Science and Engineering





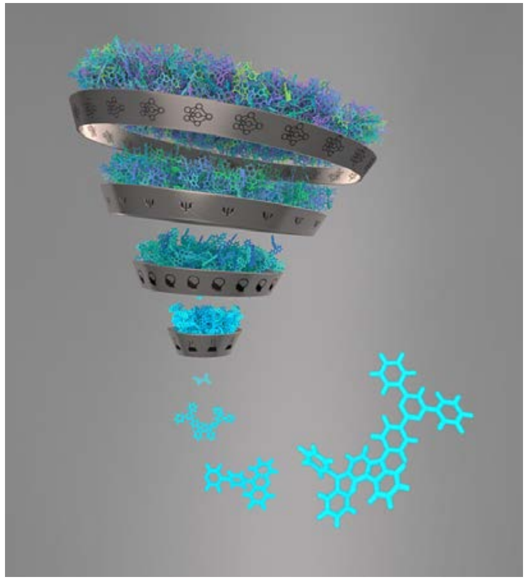
Goal: Organic Molecules for efficient light emitting diodes

Speaker today

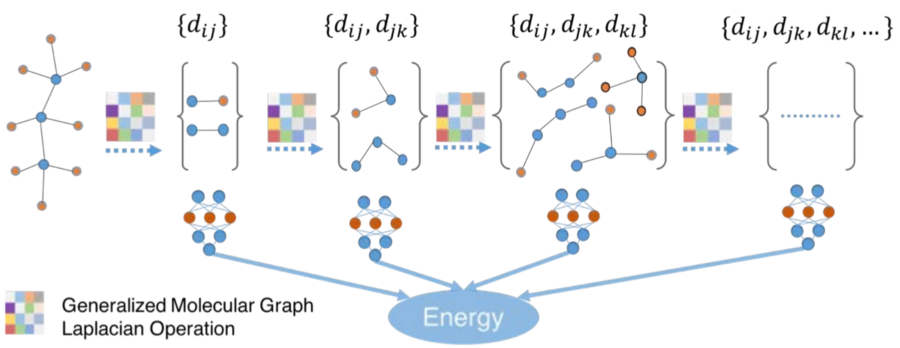
Gomez-Bombarelli et al., Nature Materials 2016

Toolset – Blurring the Lines Between Simulation and Learning

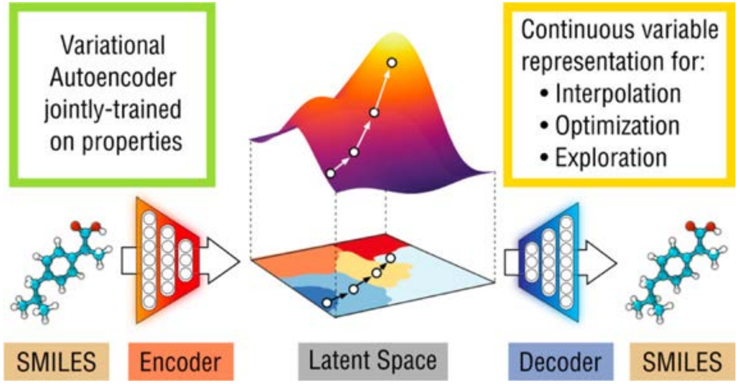
Rafael Gomez-Bombarelli, Department of Materials Science and Engineering



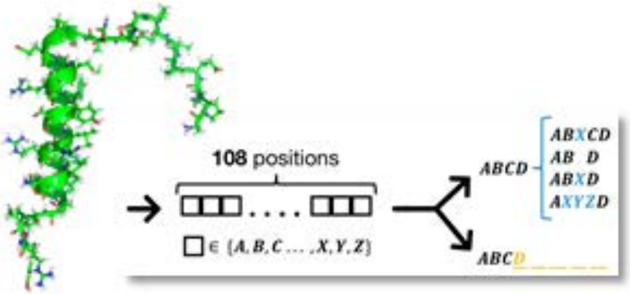
High-throughput virtual screening

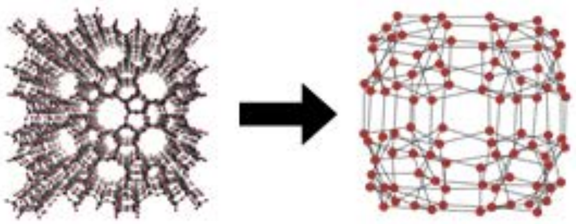


Method development / representation learning



Automatic chemical design





Data-driven discovery and optimization.

New Methods and Methodologies

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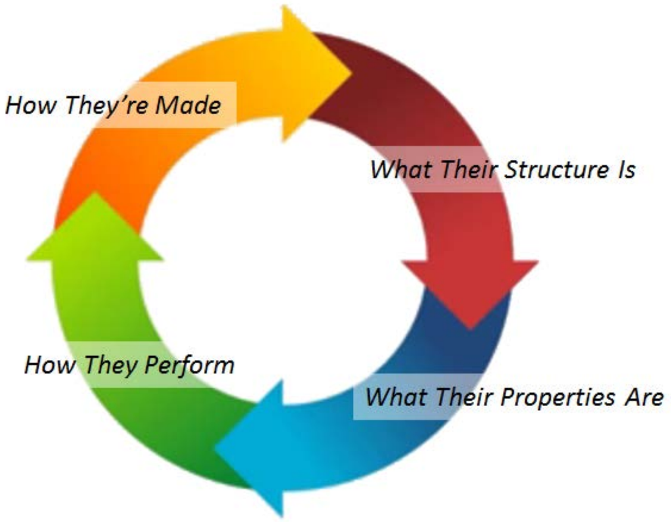

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The Materials Research Laboratory

https://mrl.mit.edu/

- Promotes Interdisciplinary Materials Research
- Provides a Nexus for Internal and External Communication
- Engages with Industry

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