THE UNIVERSITY of TENNESSEE KNOXVILLE

MACHINE LEARNING FOR MATERIALS

MSE 404/MSE504

Instructor: Sergei V. Kalinin

Times and locations: 10:20 am - 11:10 am MWF, Ferris Hall 502

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SCANNING PROBE MICROSCOPY
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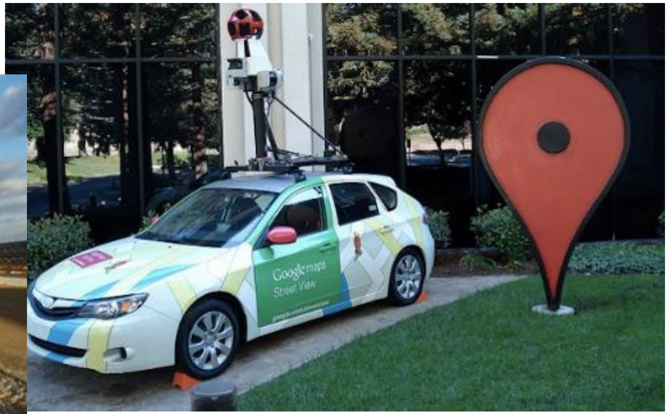
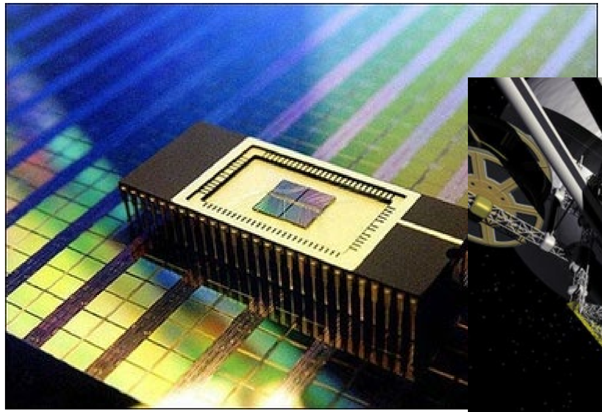
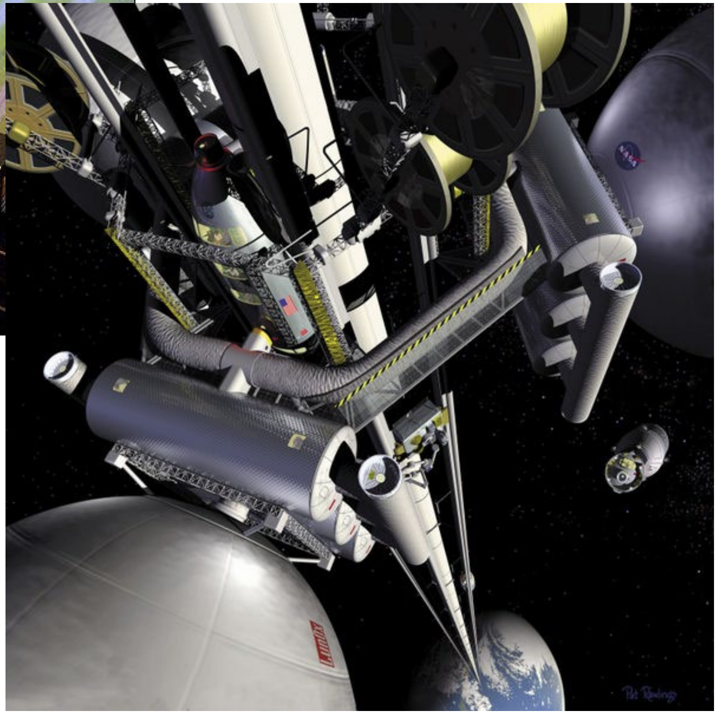
Materials Science cannot change overnight….

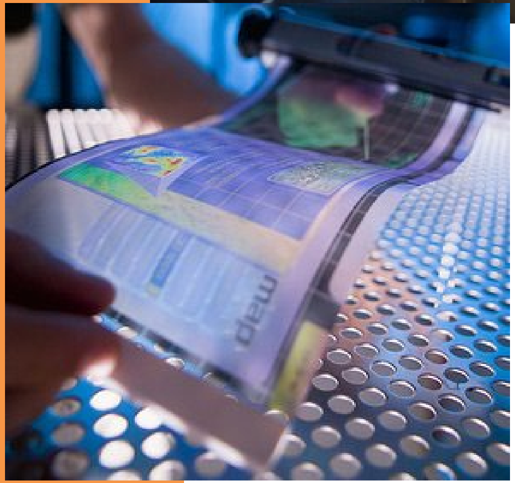
… but what is happening now comes very close

The World is Material Opportunity









Predicting crystal structure by merging data mining with quantum mechanics

CHRISTOPHER C. FISCHER[1], KEVIN J. TIBBETTS[1], DANE MORGAN[2] AND GERBRAND CEDER[1]*

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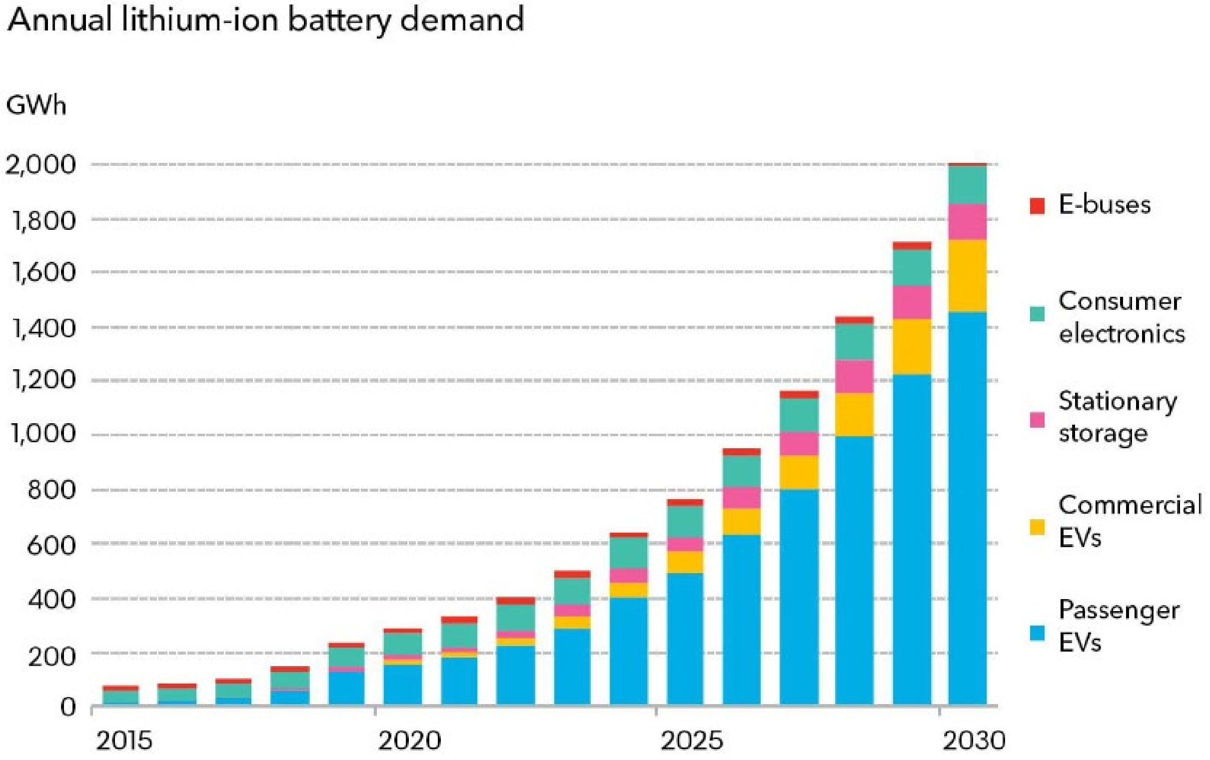
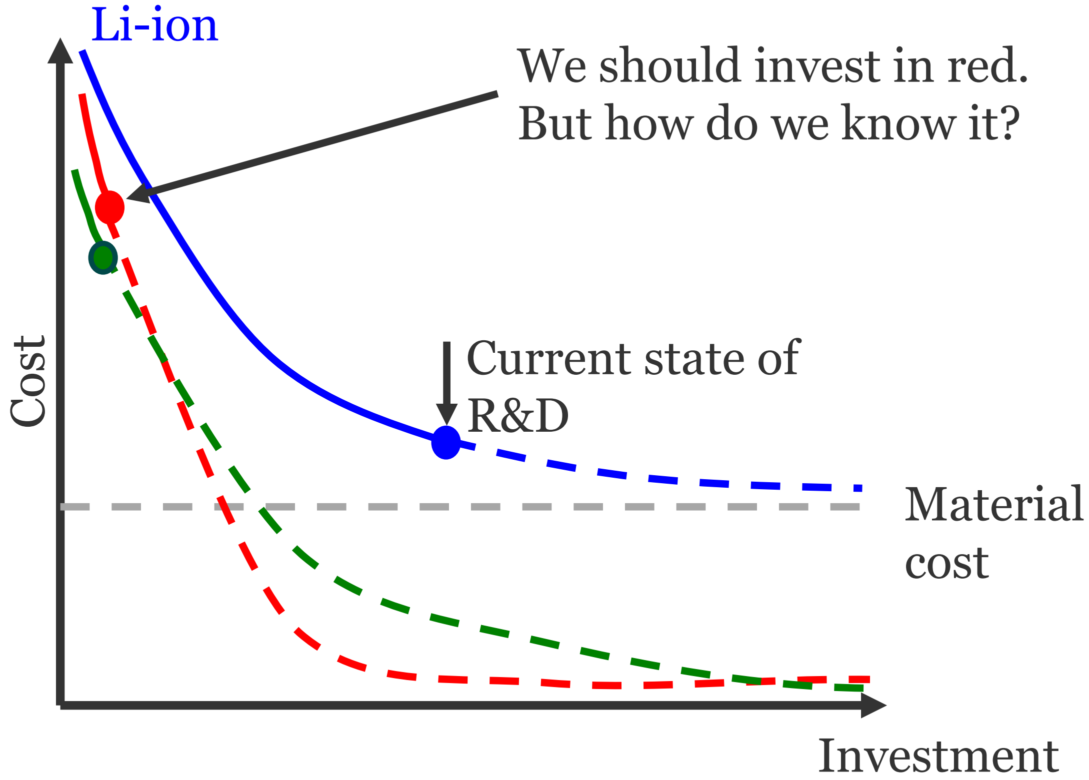
*e-mail: gceder@mit.edu

- **"Improve":** Renewable energy, self-driving cars, transparent displays, memory technologies
- **"Discover":** Room temperature superconductivity, high mechanical stress materials
- **"Engineer":** Quantum computing, single-atom catalysts, biomolecules

Functionality, manufacturability, cost

Batteries: Li-ion and Beyond

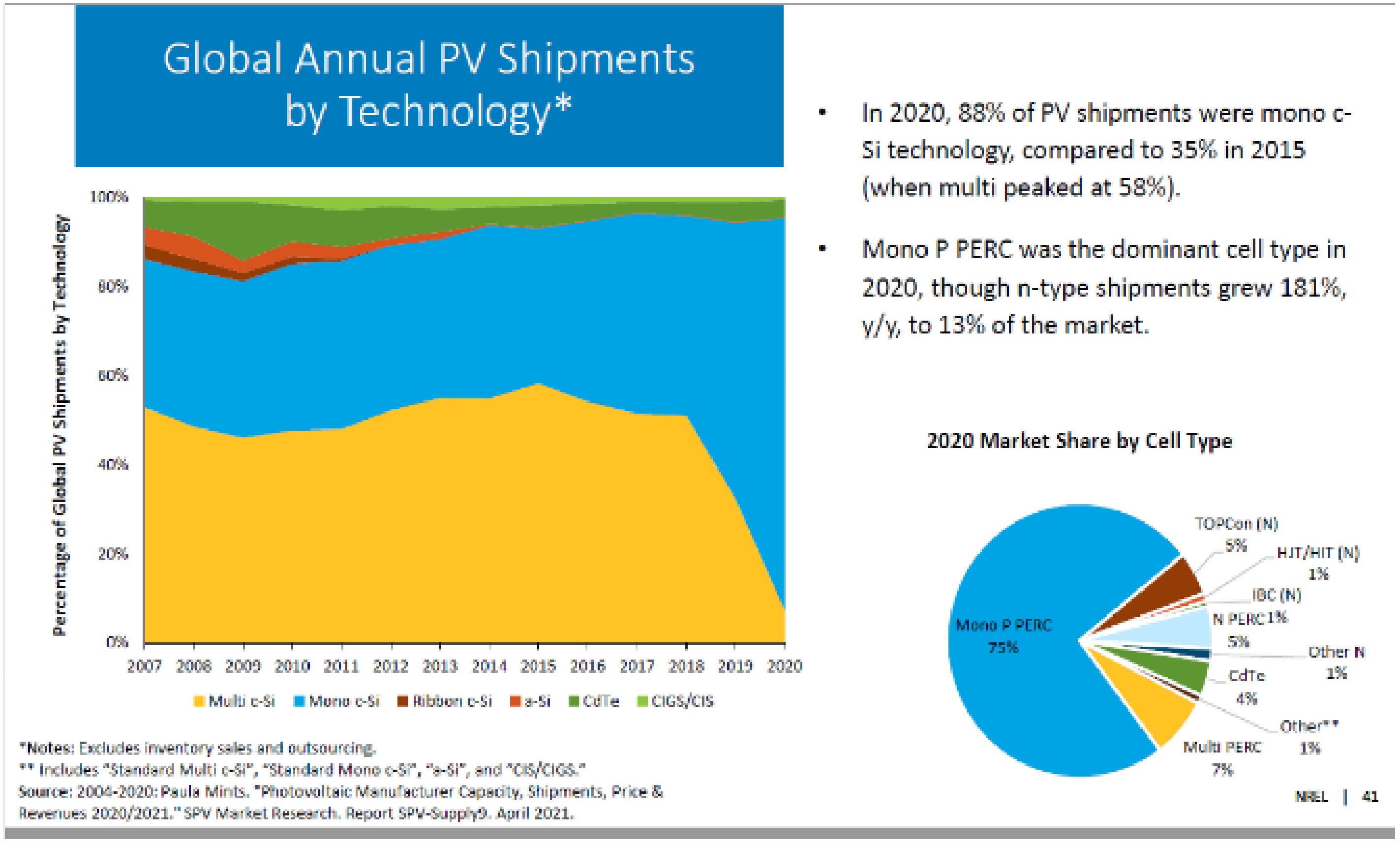


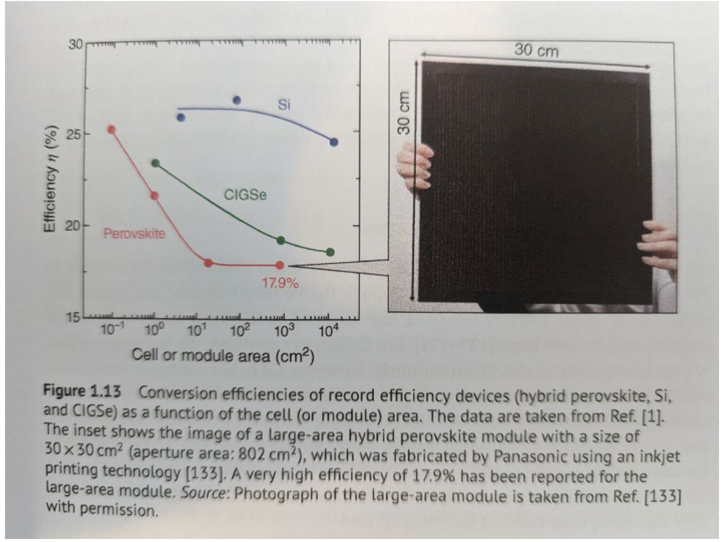


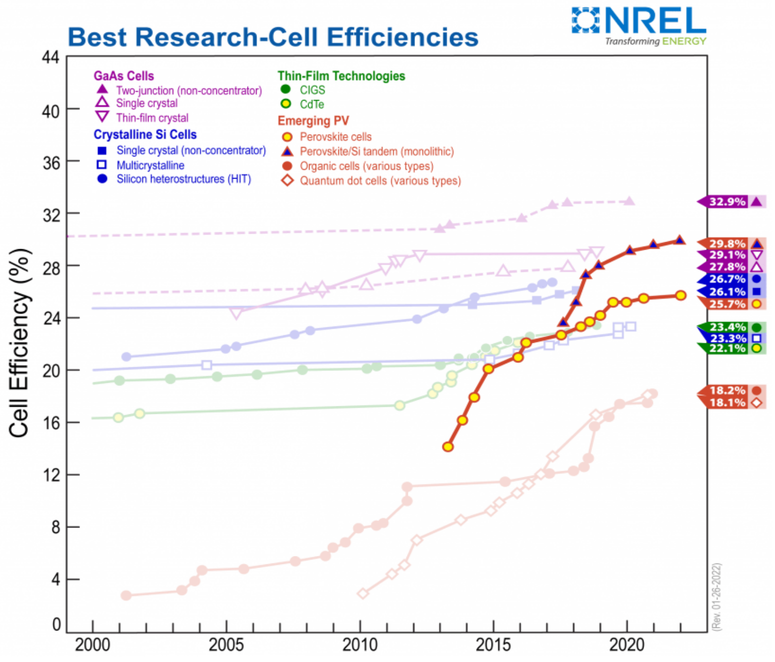
- Batteries are required element of energy transition (EVs, ESS, mobile devices)
- Currently Li-ion is the primary technology
- Optimization of Li-ion batteries takes years (even with same process on new Gigafactory)
- However, it is far from Goldilock zone for ESS or energy transport

- How can we optimize usage and safety for Li-ion batteries in EVs?
- How do we select beyond Li technologies for ESS?

Solar Energy: Will Silicon Ever Reign?

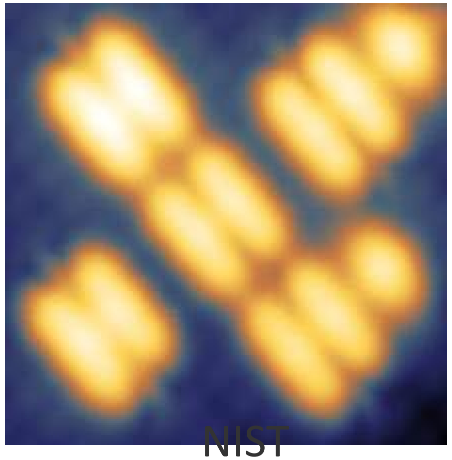




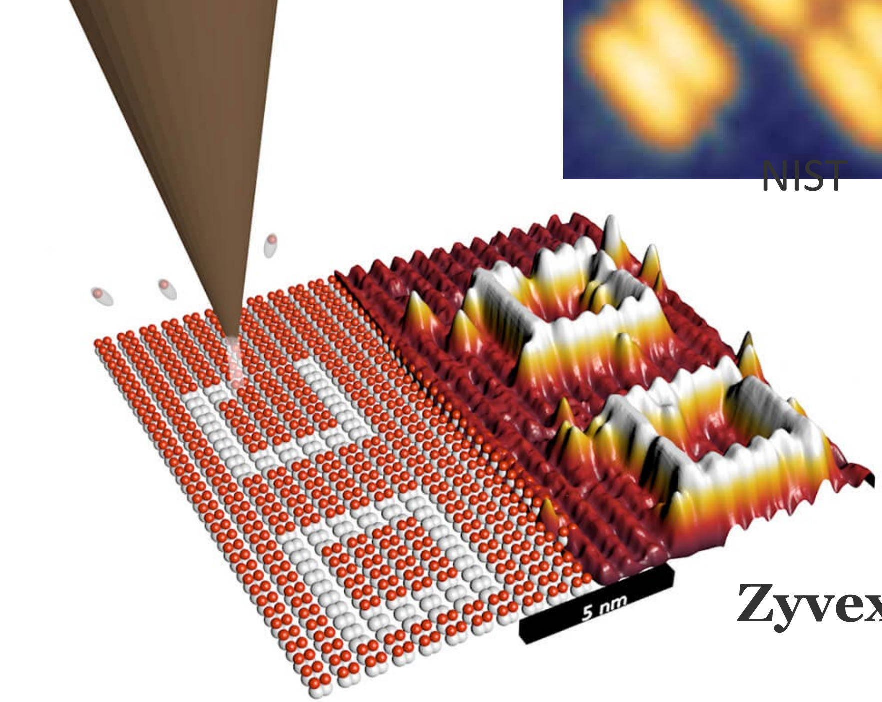


- Solar energy is the fastest growing energy sector
- Si is now reining material – however, it is really not the optimal material for PV (heavy, expensive)!
- Hybrid perovskites can be used as ideal PV materials – if we can make them stable and scale manufacturing!

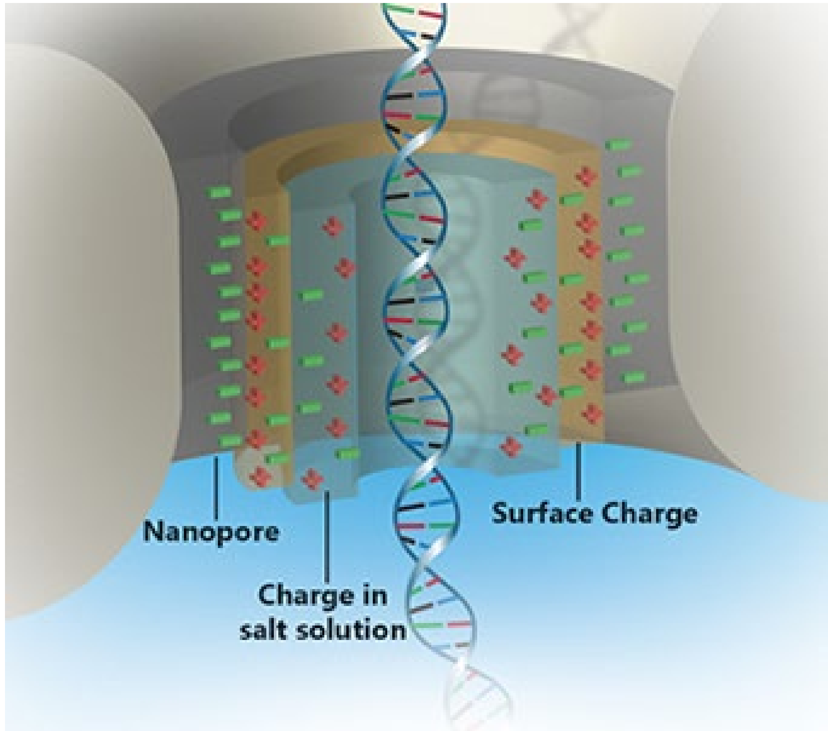
Quantum Computing and Single Molecule Bio



NIST



Zyvex Labs



Oxford Nanopore

- Direct atomic fabrication: quantum communications and quantum computing, environmental sensing
- Single-molecule biological devices

- Success story 1: cryo-electron microscopy
- Success story 2: nanoelectron diffraction

THE WHITE HOUSE

Winning the Race

AMERICA'S AI ACTION PLAN

JULY 2025

"Today, a new frontier of scientific discovery lies before us, defined by transformative technologies such as artificial intelligence... Breakthroughs in these fields have the potential to reshape the global balance of power, spark entirely new industries, and revolutionize the way we live and work. As our global competitors race to exploit these technologies, it is a national security imperative for the United States to achieve and maintain unquestioned and unchallenged global technological dominance. To secure our future, we must harness the full power of American innovation."

Donald J. Trump
45th and 47th President of the United States

https://en.wikipedia.org/wiki/Michael_Kratsios

https://en.wikipedia.org/wiki/Lynne_Parker

Introduction

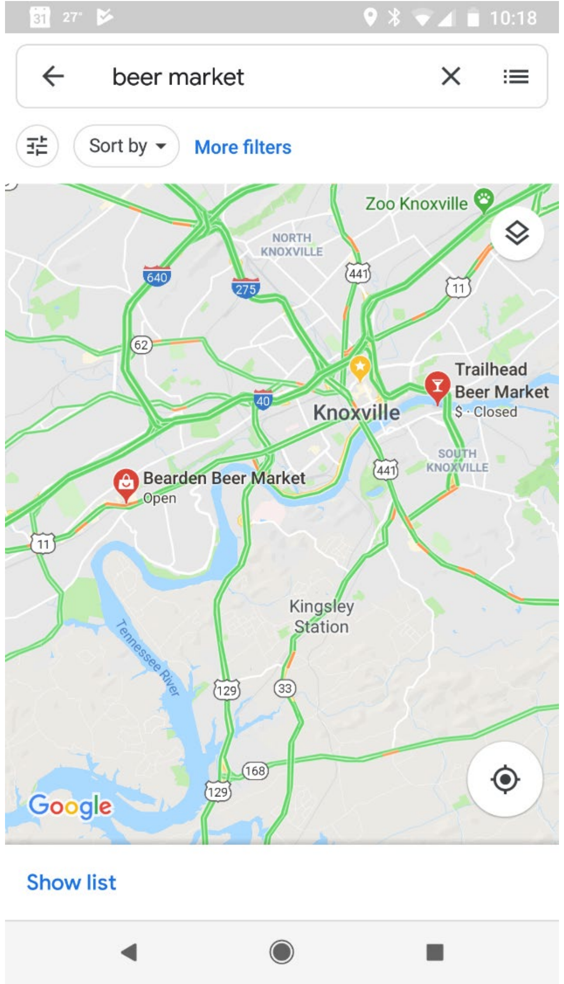
The United States is in a race to achieve global dominance in artificial intelligence (AI). Whoever has the largest AI ecosystem will set global AI standards and reap broad economic and military benefits. Just like we won the space race, it is imperative that the United States and its allies win this race. President Trump took decisive steps toward achieving this goal during his first days in office by signing Executive Order 14179, "Removing Barriers to American Leadership in Artificial Intelligence," calling for America to retain dominance in this global race and directing the creation of an AI Action Plan.[1]

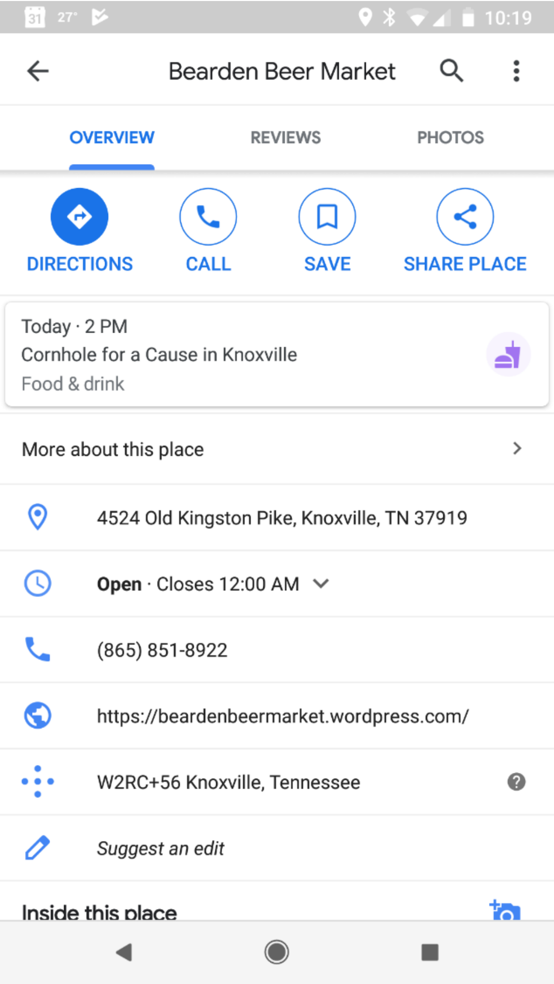
Winning the AI race will usher in a new golden age of human flourishing, economic competitiveness, and national security for the American people. AI will enable Americans to discover new materials, synthesize new chemicals, manufacture new drugs, and develop new methods to harness energy—an industrial revolution. It will enable radically new forms of education, media, and communication—an information revolution. And it will enable altogether new intellectual achievements: unraveling ancient scrolls once thought unreadable, making breakthroughs in scientific and mathematical theory, and creating new kinds of digital and physical art—a *renaissance*.

An industrial revolution, an information revolution, and a renaissance—all at once. This is the potential that AI presents. The opportunity that stands before us is both inspiring and humbling. And it is ours to seize, or to lose.

Modern day world

- Google
- Facebook
- Yelp
- Netflix
- Uber
- Lyft
- …





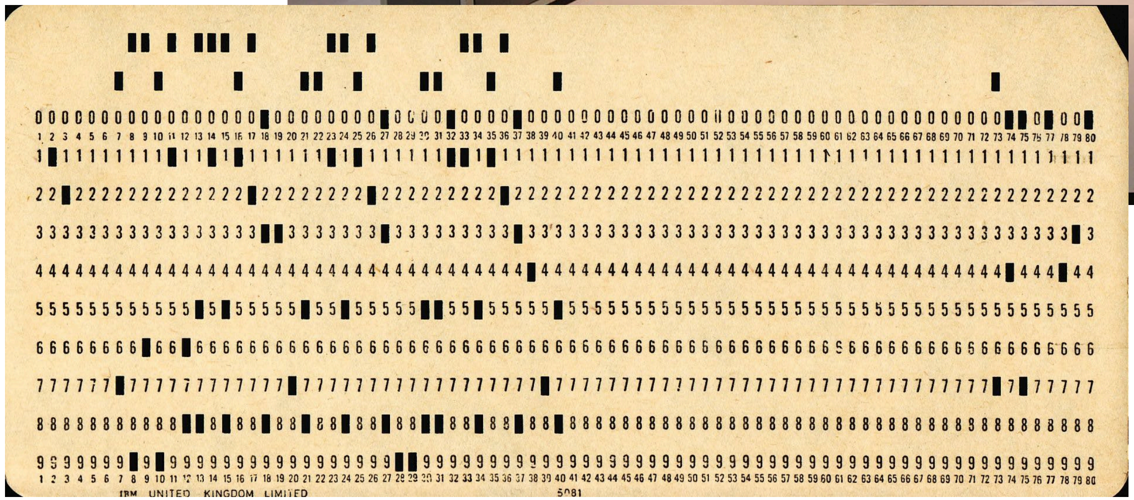
What was science like before 80ies?

- Computers existed only for specialized applications
- Many years of training before you can use one
- … and even if you can, required much patience

BESM-6 Computer

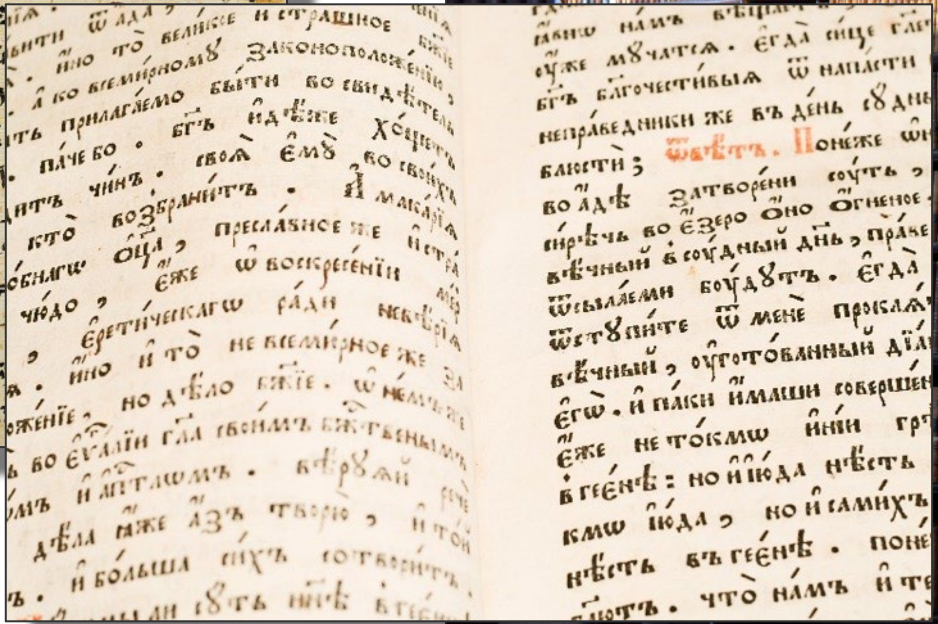
From Wikipedia

Punch card



Altair(duino)

What if you want to know more?

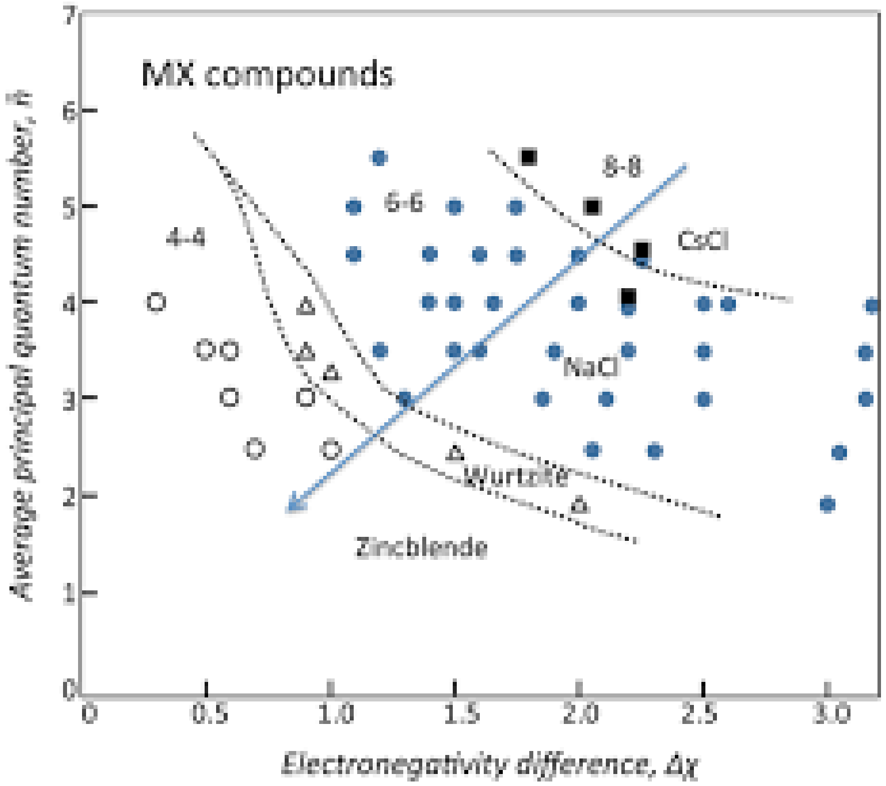


Libraries:

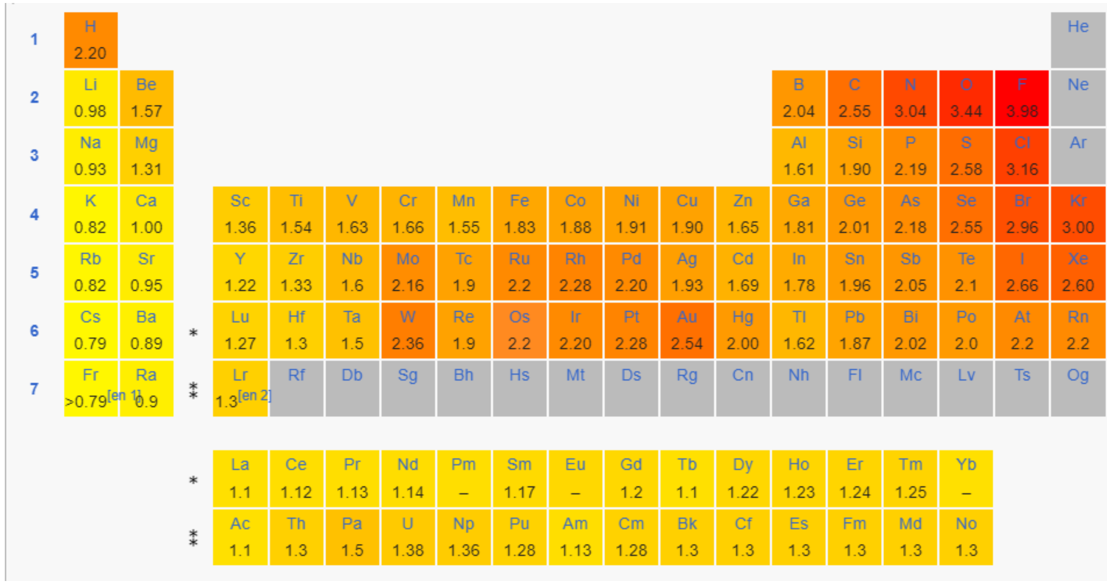
- Annual abstract books to find papers
- Dewey system to find books
- Collections: Landolt-Bornstein, etc

Was there machine learning for materials then?

Mooser-Pearson diagrams



- **Electronegativity:**



1	H 2.20																		He
2	Li 0.98	Be 1.57												B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31												Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00		Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
5	Rb 0.82	Sr 0.95		Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe 2.60
6	Cs 0.79	Ba 0.89	*	Lu 1.27	Hf 1.3	Ta 1.5	W 2.36	Re 1.9	Os 2.2	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 1.62	Pb 1.87	Bi 2.02	Po 2.0	At 2.2	Rn 2.2
7	Fr >0.79[en 1]	Ra 0.9	**	Lr 1.3[en 2]	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
			*	La 1.1	Ce 1.12	Pr 1.13	Nd 1.14	Pm –	Sm 1.17	Eu –	Gd 1.2	Tb 1.1	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb –		
			**	Ac 1.1	Th 1.3	Pa 1.5	U 1.38	Np 1.36	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3		

- **Nephelauxetic effect:**

F– < H2O < NH3 < en < [NCS - N]– < Cl– < [CN]– < Br– < N3– < I–

- **Solvent mixtures laws in organic chemistry**

Why does it matter? Physics and human heuristics is difficult to beat!

80ies

- First broadly available personal computers
- Can start programming (and get results) overnight
- First specialized scientific software
- What you have is what you bring

From Wikipedia

The 1980-2010 period:

Scientific information access:

- ISI and other data bases
- Electronic journals

General information

- Google and other search engines

Scientific software:

- Word
- Origin
- Digital micrograph

Programming languages

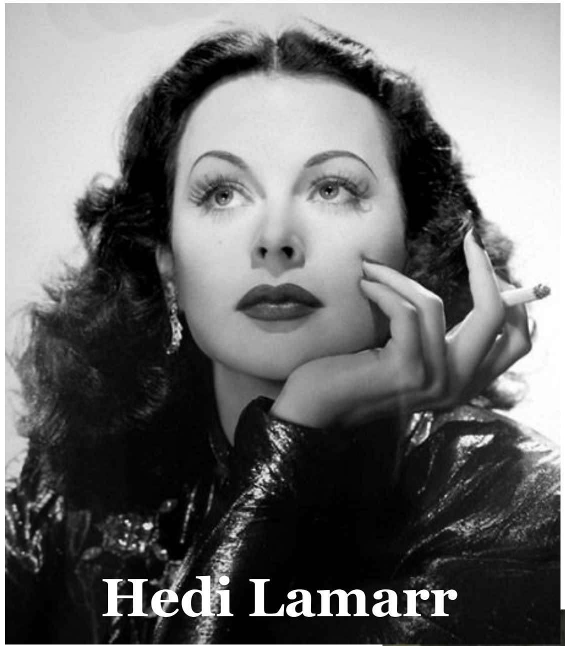
- MatLab
- Igor Pro

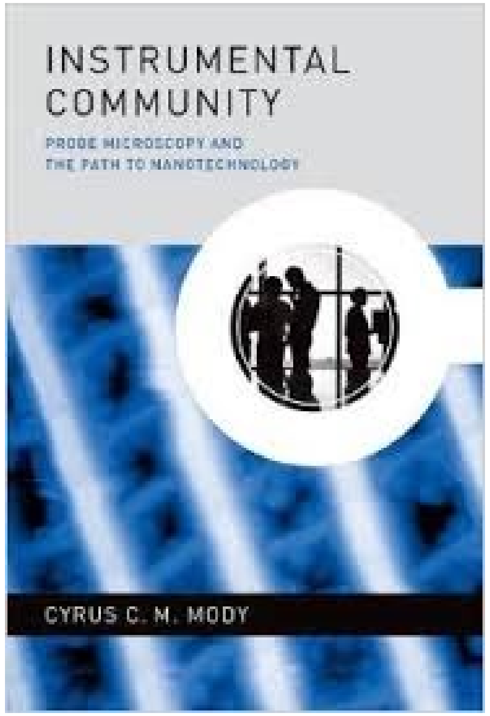
Instrument control (usually limited by manufacturer)

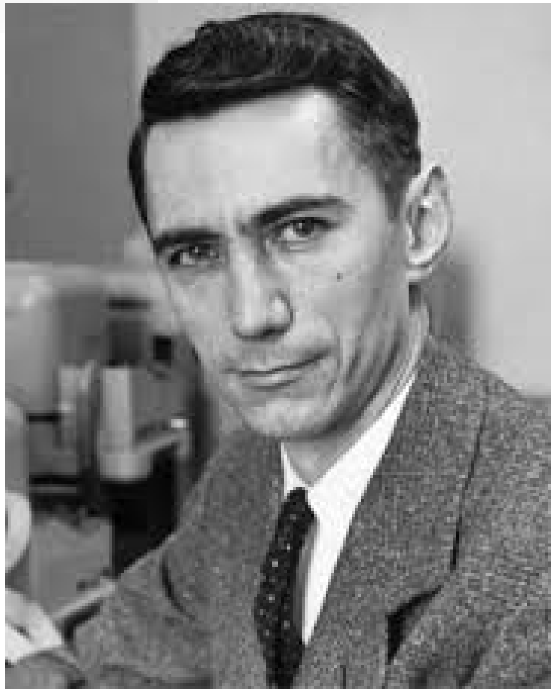
But relatively static....

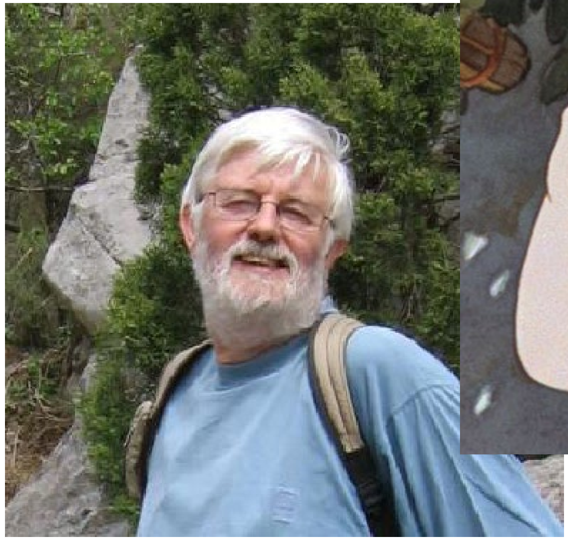
Could anyone have predicted it?


Ada Lovelace


Hedi Lamarr




Claude Shannon


Noel Bonnet

What is happening now?

New data technologies

- Searches
- Social networks
- Recommender engines
- Connection to real world
- Large Language models

New opportunities:

- 3D Printing
- IoT devices
- Laboratory robotics
- Open code
- Text analytics

The inflection point (for theory): 2006

Predicting crystal structure by merging data mining with quantum mechanics

CHRISTOPHER C. FISCHER[1], KEVIN J. TIBBETTS[1], DANE MORGAN[2] AND GERBRAND CEDER[1]*
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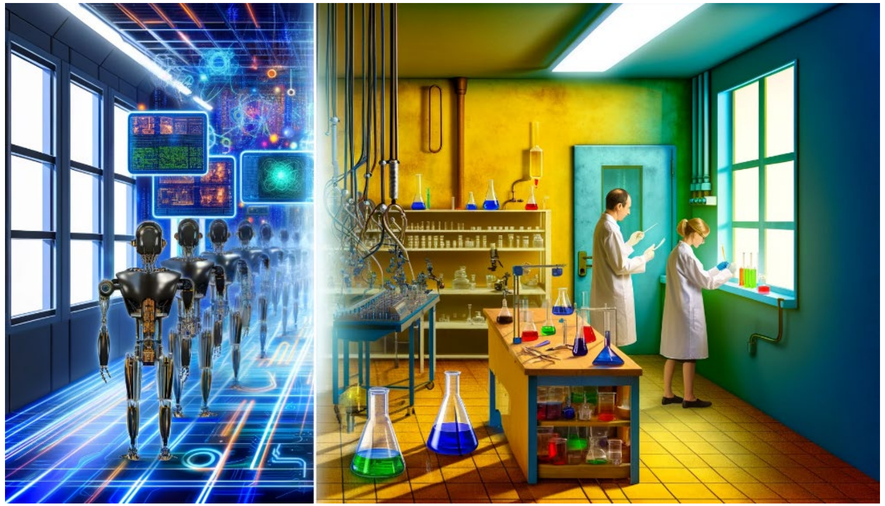
[2]Department of Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin 53706, USA
*e-mail: gceder@mit.edu

Publication by Gerd Ceder paper that is broadly seen as the inflection point launching Materials Genome Initiative in US and equivalent programs worldwide

Launch of AWS (Amazon Web Services) made cloud computing a reality – allowing businesses and scientists alike have access to computational resources without the need to build and maintain clusters

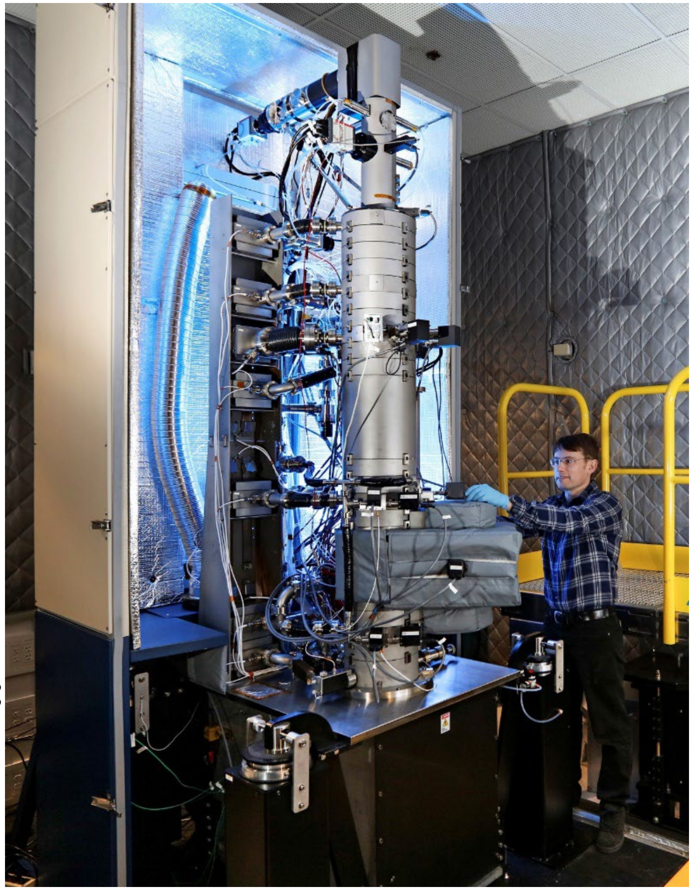


Machine learning in theory:

- Homogeneous workflows
- Known causal structure/lack of exogeneous factors
- Requires know-how, but relatively low entry barrier
- Easy to scale (given the funding)

Instrumentation

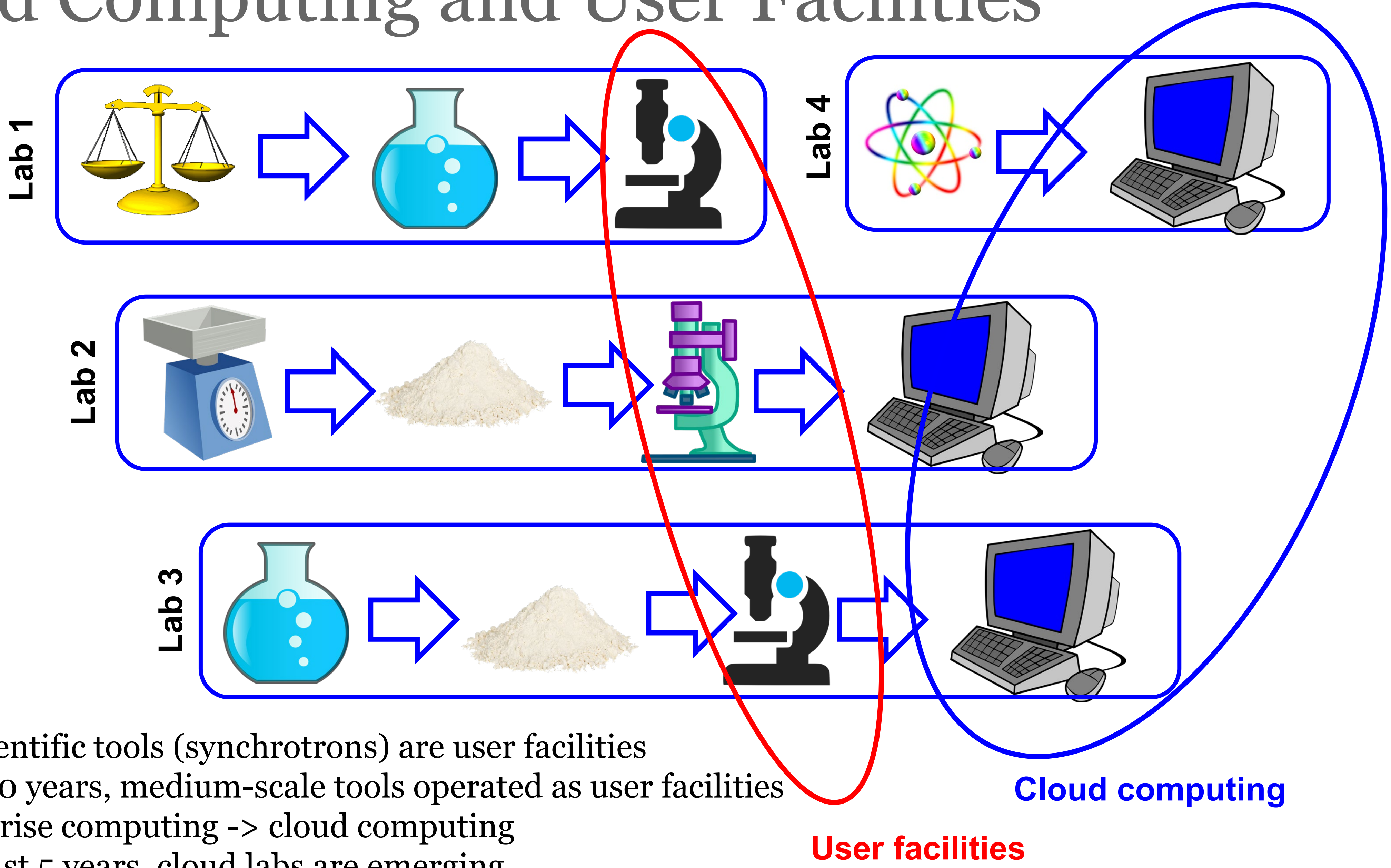
General synthesis/characterization:
- Multiple data generation tools
- Complex workflows
- 100s at each university in US



Surface science lab:
- Multiple data generation tools
- Complex controls and workflows
- 10s in each university

Electron microscope:
- >100k worldwide
- Can cost up to ~4-5$M
- Can generate data at the ~10GB/s

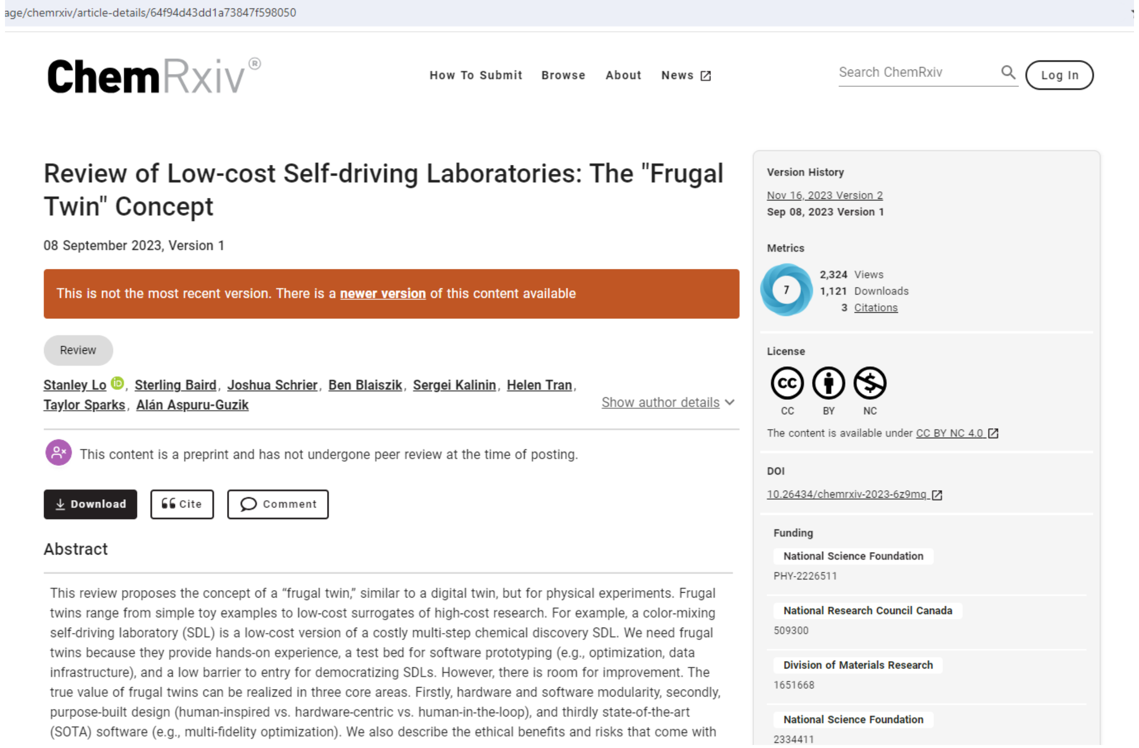
Cloud Computing and User Facilities



- Big scientific tools (synchrotrons) are user facilities
- For ~20 years, medium-scale tools operated as user facilities
- Enterprise computing -> cloud computing
- Over last 5 years, cloud labs are emerging
- What about the workflows?

The inflection point (for experiment): ~2020

- **Before 2010:** A number of (usually) confidential efforts in industry
- **2010 - 2015:** Early adopters and visionaries (Cronin, Maryama, Kusne, etc)
- **2015 – 2020:** The time of engineers
- **2020 – now:** Automated experimentation becomes broadly available with very low cost entry barriers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Review of Low-cost Self-driving Laboratories: The "Frugal Twin" Concept

08 September 2023, Version 1

This is not the most recent version. There is a newer version of this content available

Review

Stanley Lo, Sterling Baird, Joshua Schrier, Ben Blaiszik, Sergei Kalinin, Helen Tran, Taylor Sparks, Alán Aspuru-Guzik

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This content is a preprint and has not undergone peer review at the time of posting.

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Abstract

This review proposes the concept of a "frugal twin," similar to a digital twin, but for physical experiments. Frugal twins range from simple toy examples to low-cost surrogates of high-cost research. For example, a color-mixing self-driving laboratory (SDL) is a low-cost version of a costly multi-step chemical discovery SDL. We need frugal twins because they provide hands-on experience, a test bed for software prototyping (e.g., optimization, data infrastructure), and a low barrier to entry for democratizing SDLs. However, there is room for improvement. The true value of frugal twins can be realized in three core areas. Firstly, hardware and software modularity, secondly, purpose-built design (human-inspired vs. hardware-centric vs. human-in-the-loop), and thirdly state-of-the-art (SOTA) software (e.g., multi-fidelity optimization). We also describe the ethical benefits and risks that come with

Version History

Nov 16, 2023 Version 2

Sep 08, 2023 Version 1

Metrics

7

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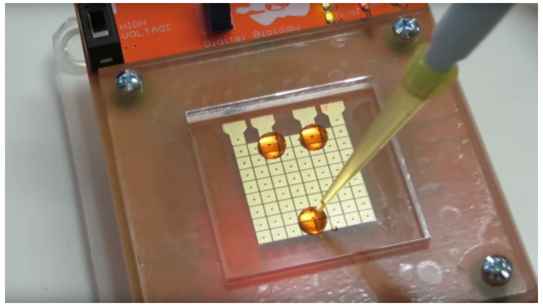
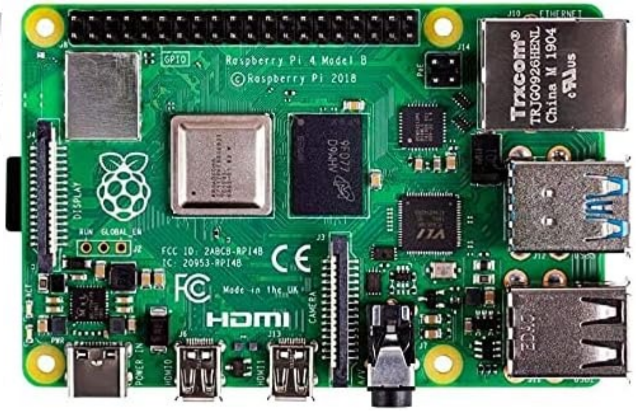
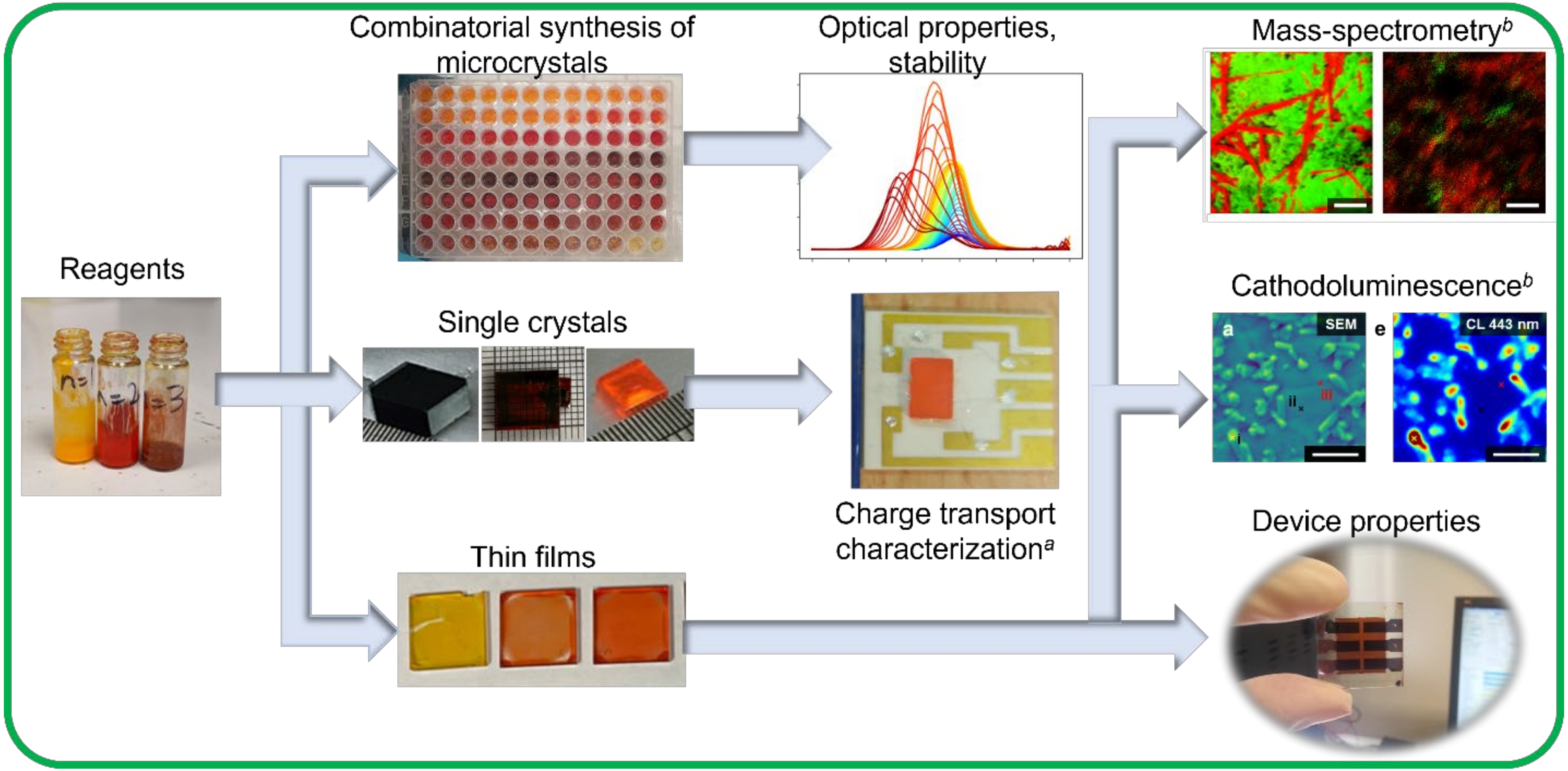




Why do we need machine learning?

To help us make decisions!

What is A Workflow?



- **Workflow:**
- Ideation, orchestration, implementation
- Domain specific language
- Dynamic planning: latencies and costs
- Reward and value functions

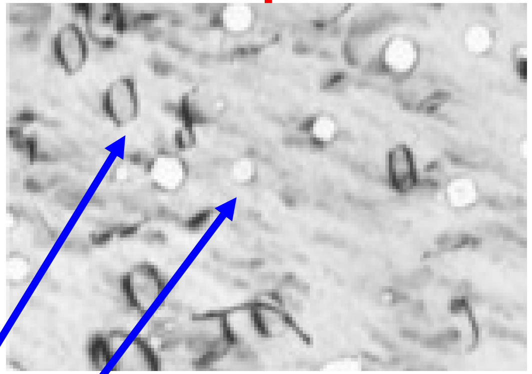
Designed in academia and adopted by industry

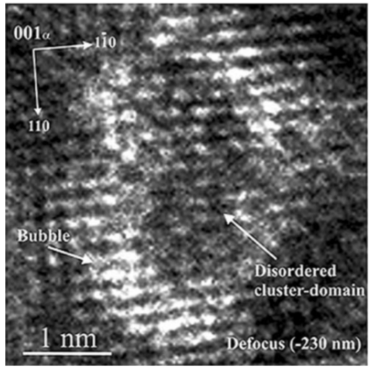
- Are they optimal?
- Can we design them better?
- Can they be changed dynamically?

Workflows for Nuclear Materials Design

Traditional experiment:
1. Always based on workflows
2. Ideated, orchestrated, and implemented by humans
3. The "gain of value" during the workflow implementation is uncertain

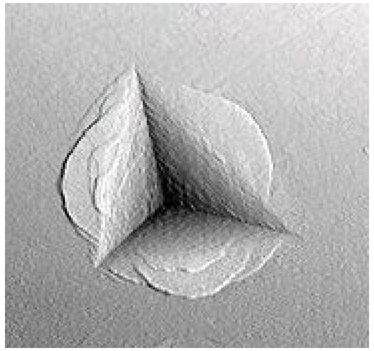
Materials selection





Prior knowledge

Operator curiosity



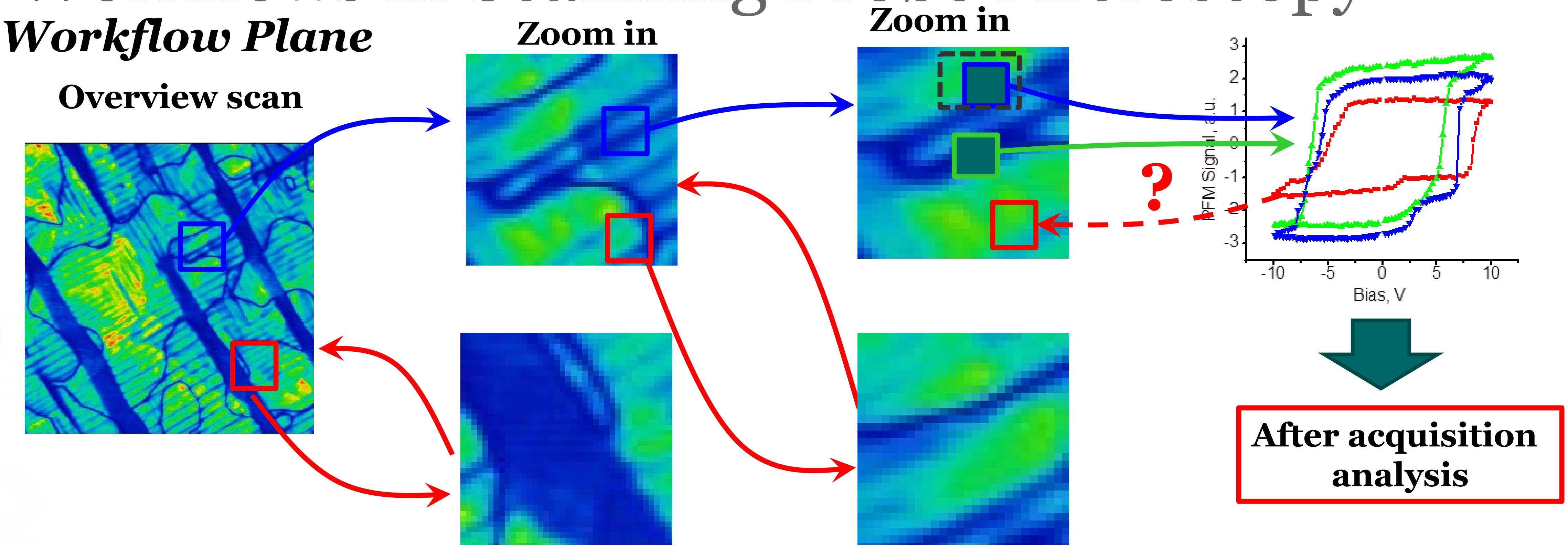
Value

Value of the step is key element:
- Either based on prior knowledge
- Or defined in a sense of the reinforcement learning Q-function

Workflows in Scanning Probe Microscopy

Workflow plane

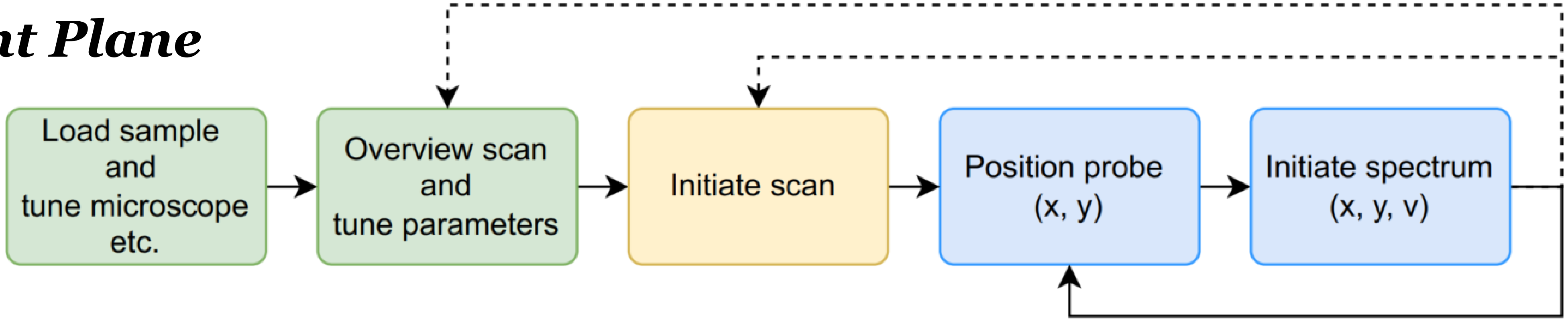
Workflow Plane



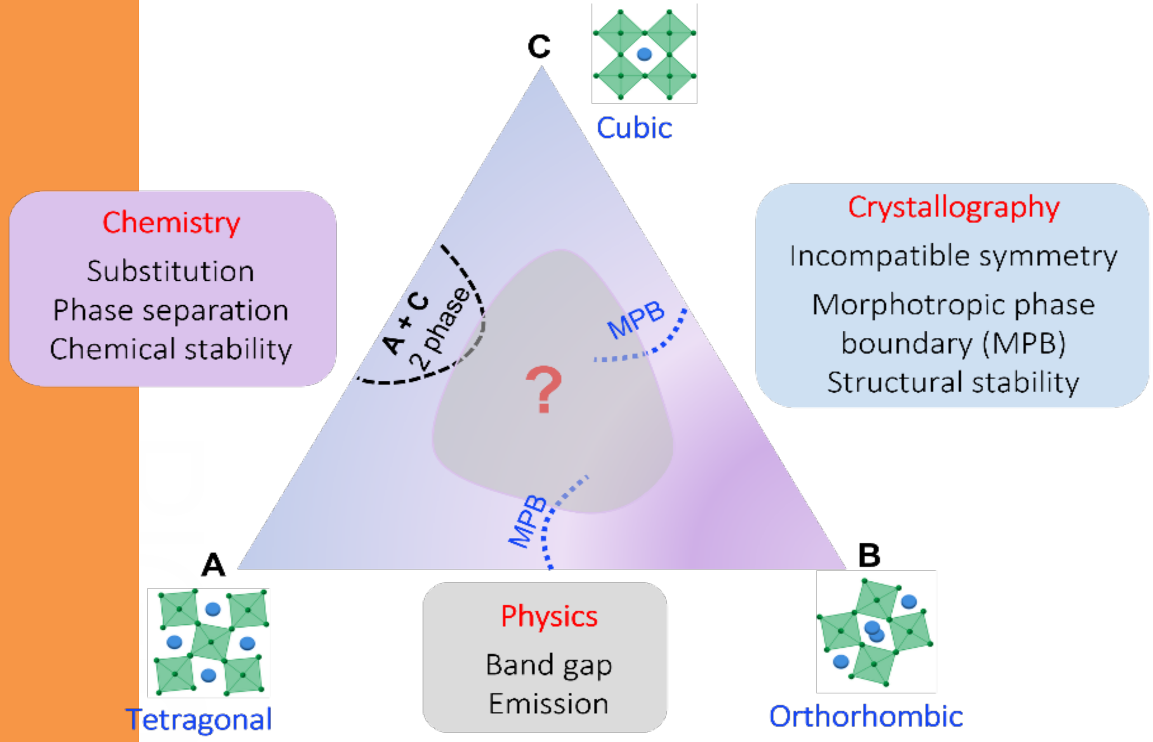
Instrument plane

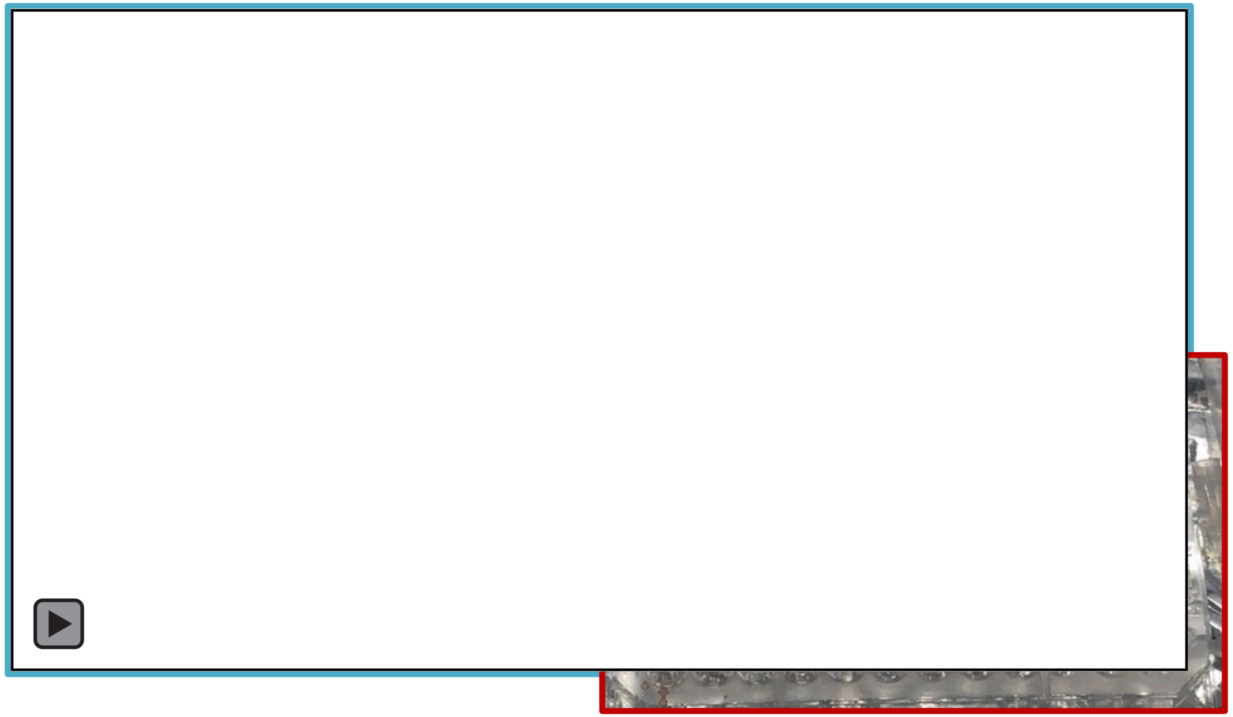
Instrument Plane

Minimal instruction set control language



Why synthesis (or theory)?

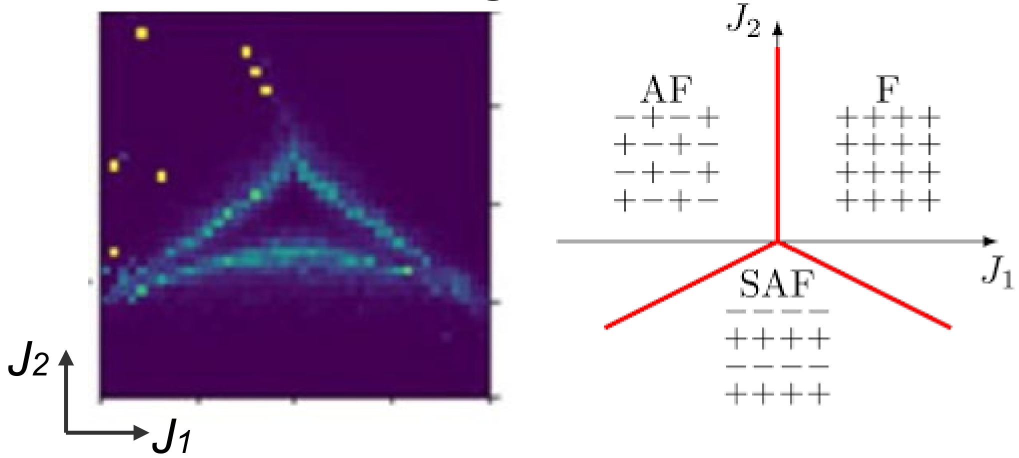




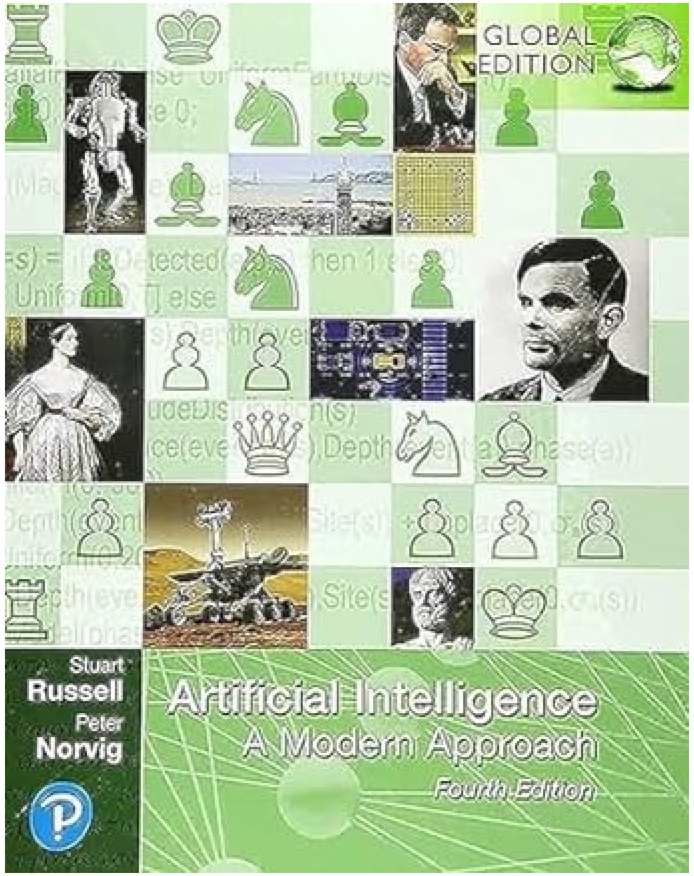
- Automated synthesis in its simplest form requires some way to navigate phase diagrams
- In more complex form, processing space.
- Ideally, incorporate physical knowledge

- Similar problem - theory

Ising model



Somewhat remarkably, almost all AI research until very recently has assumed that the performance measure can be exactly and correctly specified in the form of utility or reward function



In 2012-2014, large number of theory-trained workforce (DFT, MD, FEA) has moved into AI/ML fields

Many are returning to their original domain areas, building start-ups and corporate research centers. Many of these gain valuation very rapidly (In Silico, Schroedinger, etc)

The value created by AI/ML is orders of magnitude below investment (autonomous driving, radiology, cashier less stores)

Real-world industries and manufacturing are looking for work force with the combination of **domain** and **ML/AI** expertise

Course Information

Faculty Contact Information:

Instructor:	Prof. Sergei V. Kalinin,
Office:	314 IAMM
E-mail:	sergei2@utk.edu
Teaching Assistant:	Aditya Raghavan, araghav4@vols.utk.edu

Instructor Availability:
Please don't hesitate to email me with updates, questions, or concerns. I will typically respond within 24 hours during the week and 48 hours on the weekend. I will notify you if I will be out of town and if connection issues may delay a response.

Meeting Time: 10:20 am - 11:10 am MWF, Ferris Hall 502

The lectures and materials will be posted on Canvas and at GitHub:
https://github.com/SergeiVKalinin/MSE_Fall2025

Office Hours:
Friday 1:30 - 3:00 PM are open for 1:1 meetings to discuss any course related item. Please set up time via email.

Prerequisites

To be successful in this course you will need a general background in materials science. Python or similar programming experience, while not essential, will be extremely useful. Students without any prior programming experience should expect to spend extra time outside of class learning basic skills.

This and that

Learning Environment:
The class will be delivered as in-person lectures. The Jupyter notebooks, code libraries, and videos provided. Weekly programming exercises will be assigned via Google Colabs and those students wishing to interact with the instructor in person should attend office hours.

Use of ChatGPT:
Strongly encouraged both for programming and written assignments. However, the students have to be aware of the limitations of the generative models.

Grading & Policies:

• Homework assignments	40%
• Mid-terms (2)	30%
• Final Project & Presentation	30%

Reference Materials

I will provide copies of lecture notes, presentations, and Colabs on GitHub and Canvas. There is no specific textbook for the course and we will take material from a variety of sources including:

- Andrew Bird et al, *Python Workshop – Second Edition*, https://subscription.packtpub.com/book/programming/9781804610619/1

- Sebastian Raschka, *Machine Learning with PyTorch and Scikit-Learn*, https://subscription.packtpub.com/book/data/9781801819312/1

- Rowel Atienza, *Advanced Deep Learning with TensorFlow 2 and Keras - Second Edition*, https://www.packtpub.com/product/advanced-deep-learning-with-tensorflow-2-and-keras-second-edition/9781838821654

- (Optional) Alaa Khamis, Optimization Algorithms: AI Techniques for Design, Planning, and Control Problems, https://www.manning.com/books/optimization-algorithms

- (Optional) Peter Norvig, Artificial Intelligence: A Modern Approach, Global Edition, https://www.amazon.com/Artificial-Intelligence-Modern-Approach-Global/dp/129240113

Homework 1:

- Create new Colab, https://colab.google/
- Explore NotebookLM, https://notebooklm.google/
- Chapter 1-4, Python Workshop.