“Machine learning” – what comes to mind?

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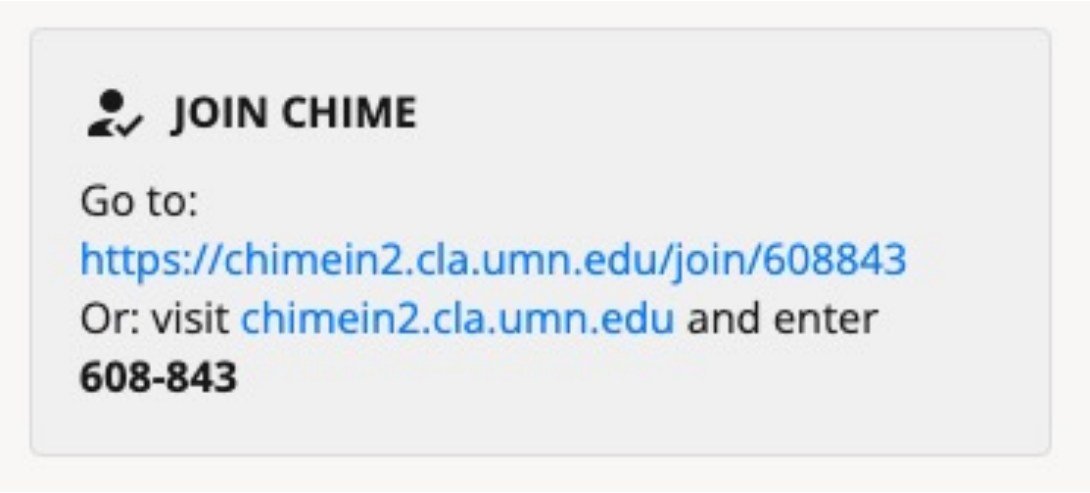

Data Science vs AI vs ML

Data science → extract insights from data

- Machine learning → make predictions w/o explicit programming
- AI → systems that automatically do human-like things

“Large language model” enters the lexicon

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CNN

How good is ChatGPT?

Millions have been using the new AI technology ChatGPT for everything from songwriting to this CNN commentary. "It's good for people trying...

8 hours ago

“Large language model” enters the lexicon

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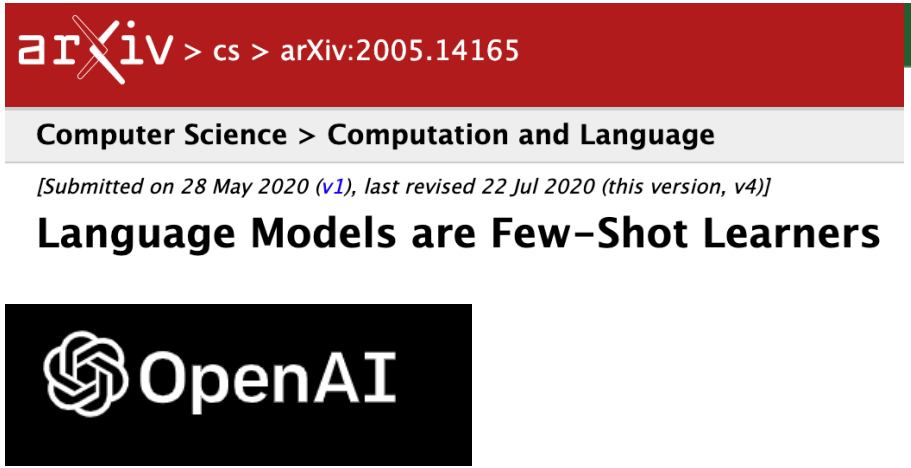

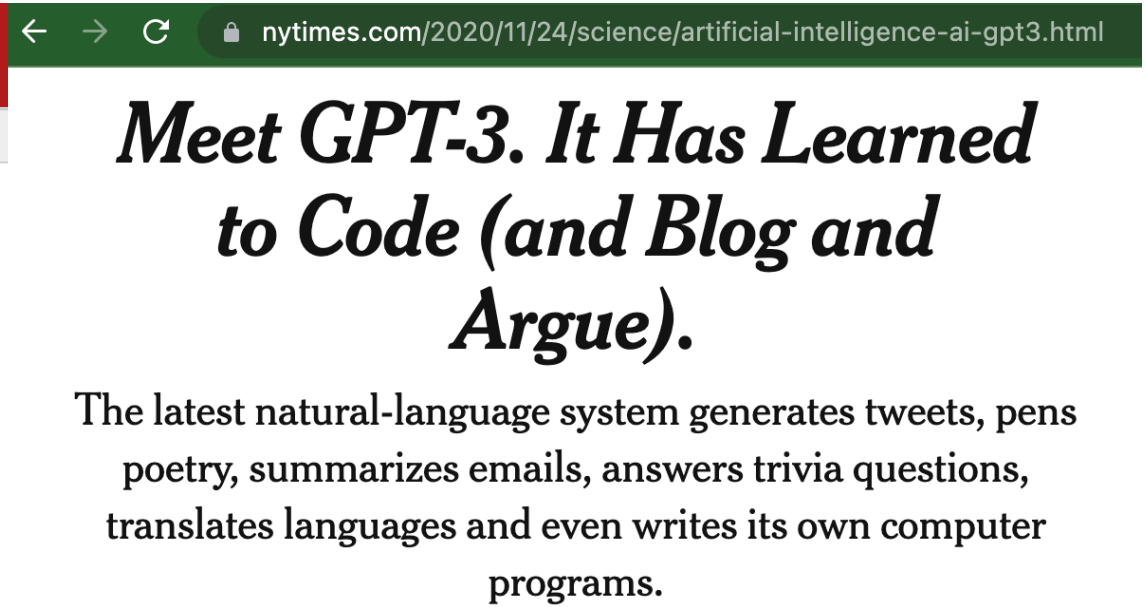

Let’s try it out!

https://chat.openai.com/

ML advances not without controversy

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NBC News

ChatGPT used by mental health tech app in AI experiment with users

ChatGPT was used by the emotional support chat app Koko to write responses for real users. Controversy came quickly after the experiment was...

9 hours ago

ML advances not without controversy

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The Washington Post

Analysis | Our Future Artificial Intelligence Overlords Need a ··· Resistance Movement

Artificial intelligence has been moving so fast that even the scientists are finding it hard to keep up. In the past year, machine learning...

47 mins ago

ML advances not without controversy

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Gizmodo

AI Image Generators Routinely Display Gender and Cultural Bias

AI Image Generators Routinely Display Gender and Cultural Bias ... Artificial intelligence researcher for Hugging Face, Sasha Luccioni,...

2 days ago

The Hill

Common AI language models show bias against people with disabilities: study

New research underscores the implicit bias present in some artificial intelligence language models. Researchers found models were generally...

3 weeks ago

And challenges!

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Bloomberg.com

Even After $100 Billion, Self-Driving Cars Are Going Nowhere

The first car woke Jennifer King at 2 a.m. with a loud, ... who studies artificial intelligence and the limits of self-driving vehicles.

1 month ago

The Washington Post

MIT scientists find self-driving cars might be harmful to the climate

MIT researchers found that the computers powering self-driving cars could have a large carbon footprint.

2 days ago

But also successes!

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Predicted the spread of the winter flu outbreak in 2009 in the USA down to the state level.

Search query topics that were highly correlated with flu outbreaks

- Influenza complication
- Cold/flu remedy
- General influenza symptoms
- Term for influenza
- Specific influenza symptom
- Symptoms of an influenza complication
- Antibiotic medication
- General influenza remedies
- Symptoms of a related disease
- Antiviral medication
- Related disease

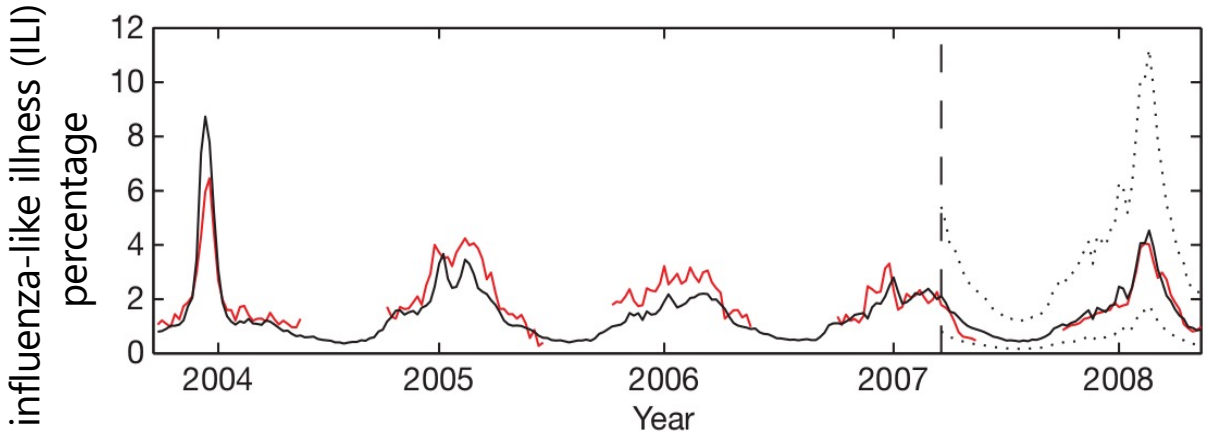


Figure 2 | A comparison of model estimates for the mid-Atlantic region (black) against CDC-reported ILI percentages (red), including points over which the model was fit and validated.

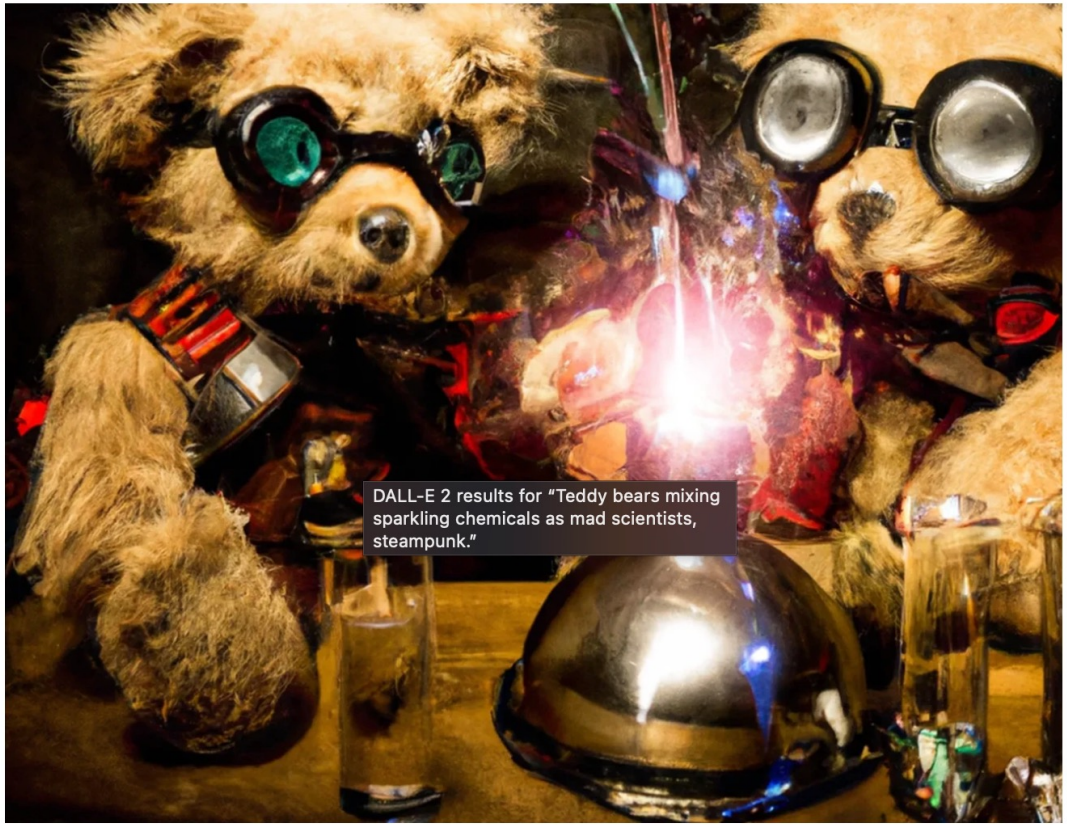
Google took 50 million of the most common searches and compared them to the CDC data on the spread of the winter flu from 2003 to 2008. Ginsberg *et al.* Nature (2009).

But also successes!

https://deepmind.com/research/alphago/; doi:10.1038/nature16961 (also on Netflix!)

First ML for games → Samuel, Arthur L. "Some studies in machine learning using the game of checkers." *IBM Journal of research and development* 3.3 (1959): 210-229.

But also successes!



DALL-E 2 results for “Teddy bears mixing sparkling chemicals as mad scientists, steampunk.”

But also successes!

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PERSPECTIVE

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Cite this: *Digital Discovery*, 2022, 1, 79

Natural language processing models that automate programming will transform chemistry research and teaching†

Glen M. Hocky *[a] and Andrew D. White *[b]

```
"""
Compute the dissociation curve of H2 using the pyscf library
"""
```

But also successes!

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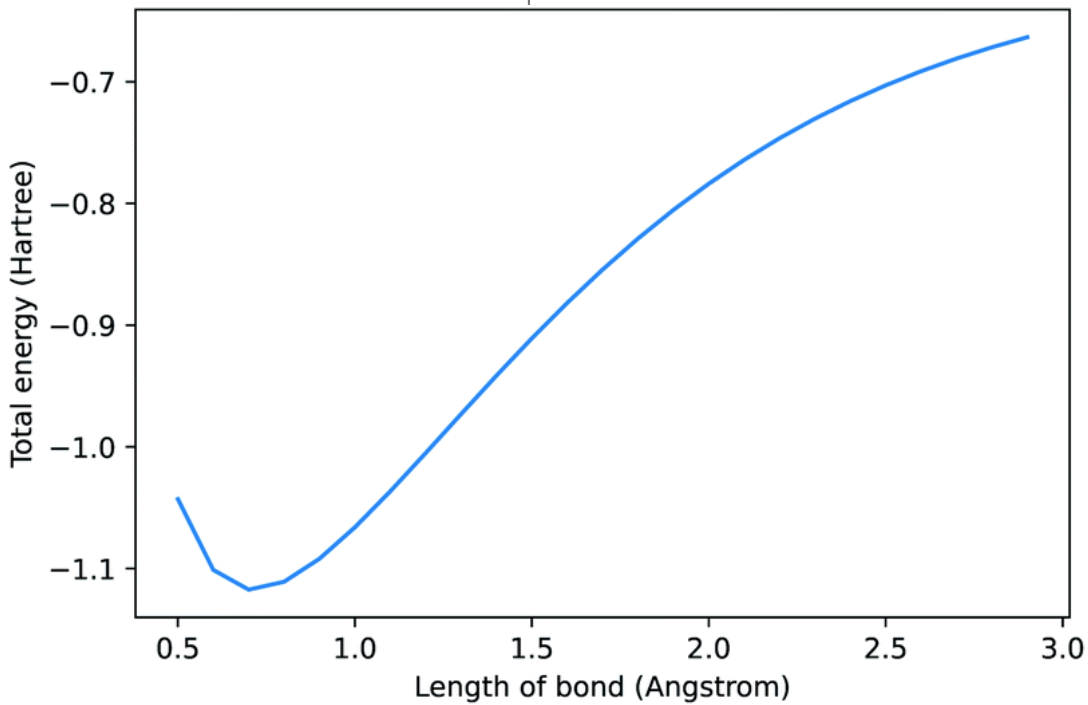
```
"""
Compute the dissociation curve of H2 using the pyscf library
"""
import numpy as np
import pyscf
from pyscf import gto, scf, dft

# Define the molecule
mol = gto.M(atom='H 0 0 0; H 0 0 1.4', basis='sto-3g', verbose=3)

# Compute the reference energy
en_ref = mol.energy_nuc()

# Compute the dissociation curve
r = np.linspace(0.5, 2.0, 100)
en = []
for b in r:
    mol.atom = [['H', (0, 0, 0)], ['H', (0, 0, b)]]
    mol.build()
    mf = scf.RHF(mol)
    mf.kernel()
    en.append(mf.e_tot - en_ref)

# Plot the dissociation curve
import matplotlib.pyplot as plt
plt.plot(r, en)
plt.xlabel('Bond length (Bohr)')
plt.ylabel('Energy (Hartree)')
plt.show()
```



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Natural language processing models that automate programming will transform chemistry research and teaching†

Glen M. Hocky *a and Andrew D. White *b

But also successes!

Article | Open Access | Published: 05 October 2022

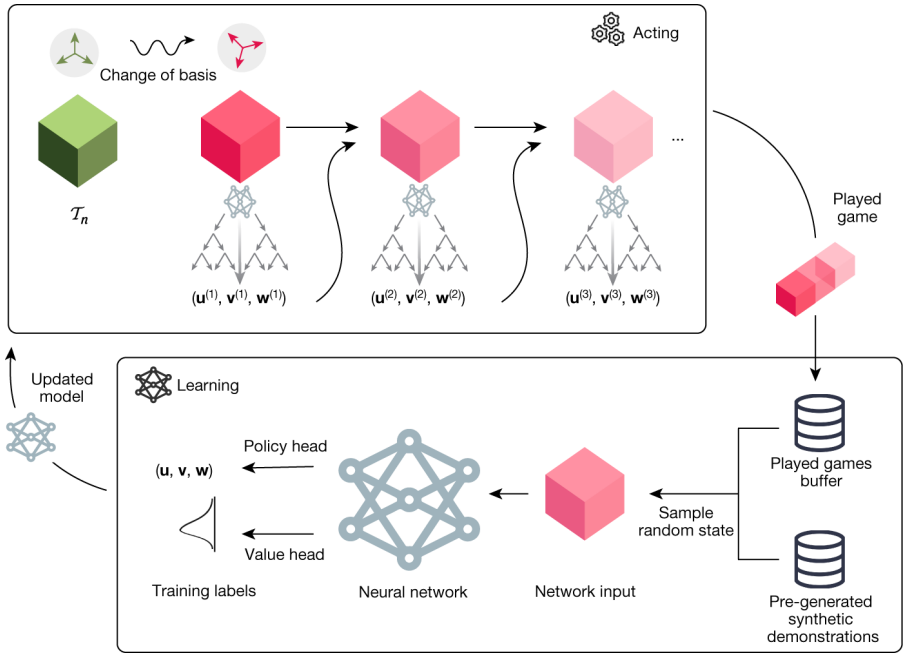
Discovering faster matrix multiplication algorithms with reinforcement learning

Alhussein Fawzi ✉, Matej Balog, Aja Huang, Thomas Hubert, Bernardino Romera-Paredes, Mohammadamin Barekatain, Alexander Novikov, Francisco J. R. Ruiz, Julian Schrittwieser, Grzegorz Swirszcz, David Silver, Demis Hassabis & Pushmeet Kohli

Nature **610**, 47–53 (2022) | Cite this article

460k Accesses | **3** Citations | **3642** Altmetric | Metrics

the-art complexity for many matrix sizes. Particularly relevant is the case of 4 × 4 matrices in a finite field, where AlphaTensor's algorithm improves on Strassen's two-level algorithm for the first time, to our knowledge, since its discovery 50 years ago[2]. We further showcase the



Faster matrix multiplication → less computational time for trillions of calculations…
Fawzi *et al.* Nature (2022).

How about in the Computational Molecular Sciences?

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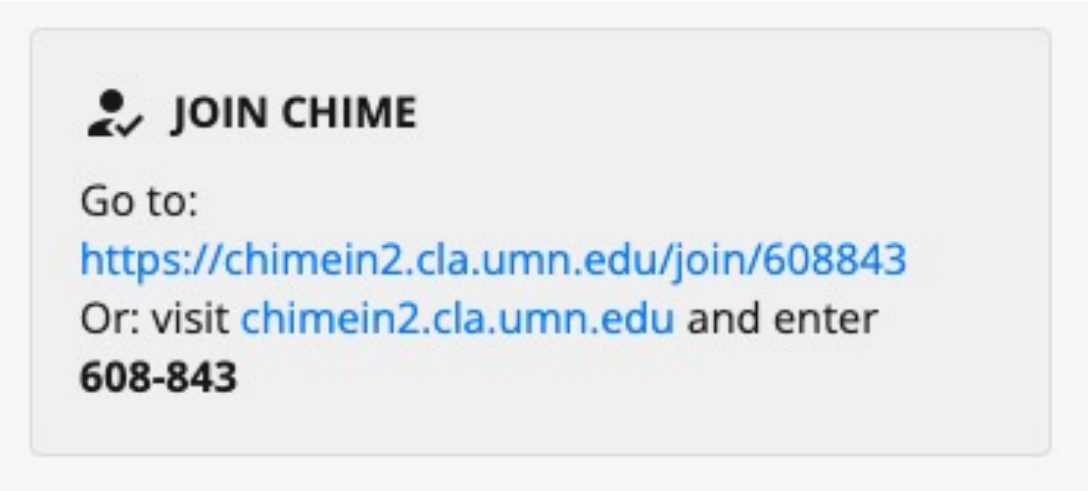

ML in Computational Molecular Sciences

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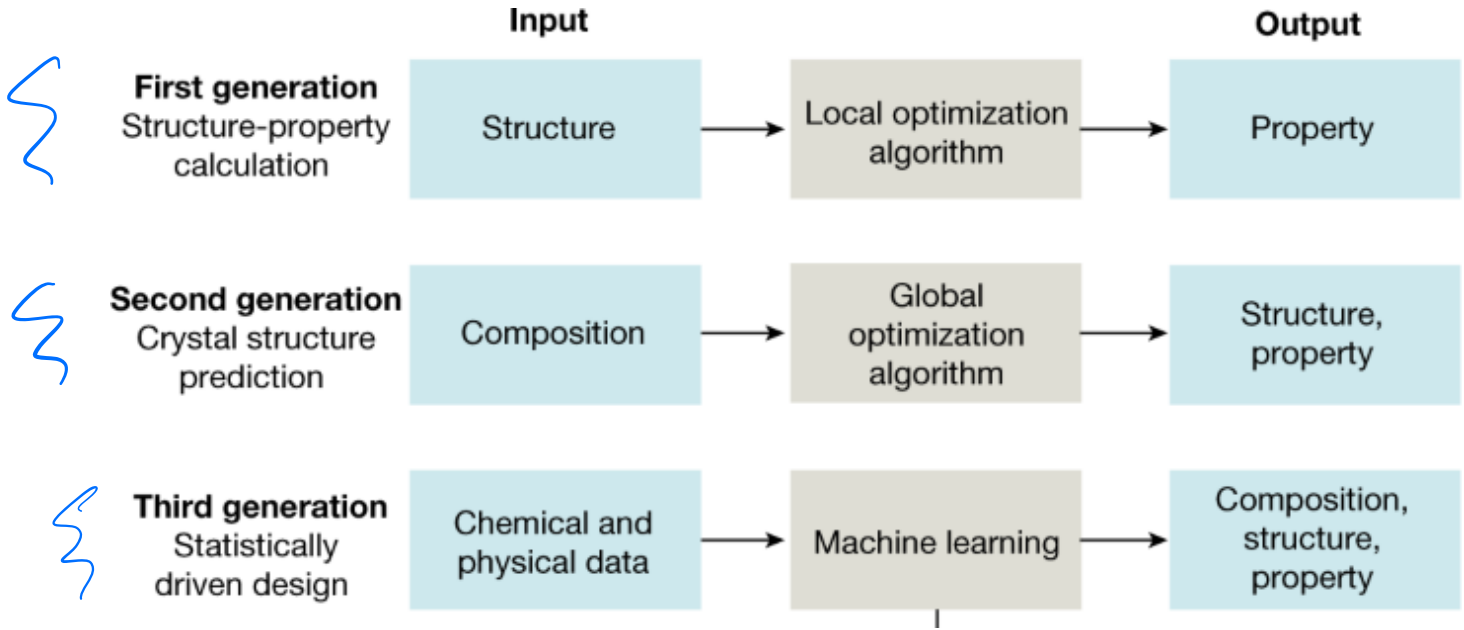
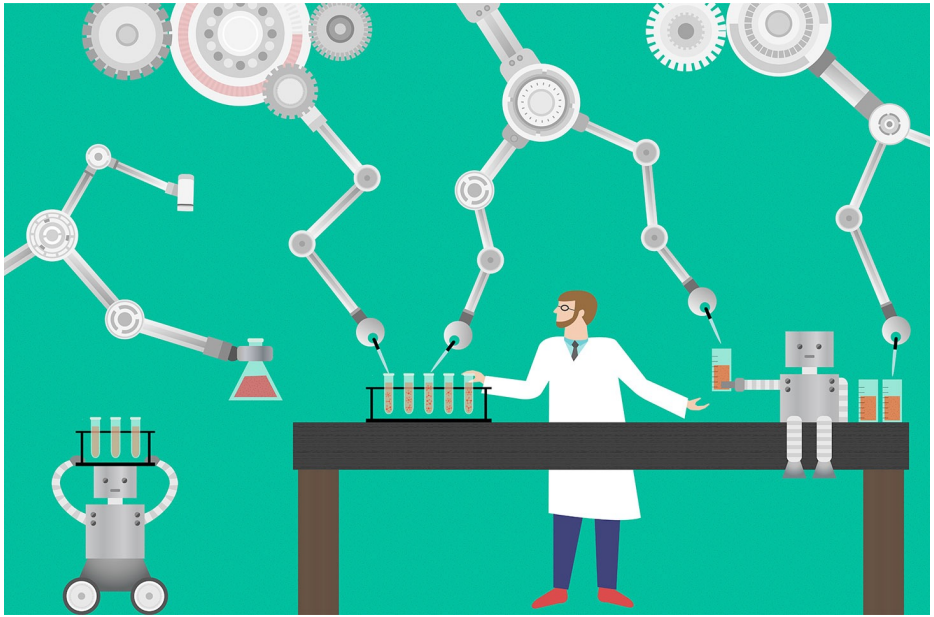


Butler et al. "Machine learning for molecules and materials science." *Nature* (2021).

ML in Computational Molecular Sciences



Kitchin, John R. "Machine learning in catalysis." *Nature Catalysis* (2018).

FACEBOOK AI Carnegie Mellon University

Open Catalyst Project

Using AI to model and discover new catalysts to address the energy challenges posed by climate change.

opencatalystproject.org

ML in Computational Molecular Sciences

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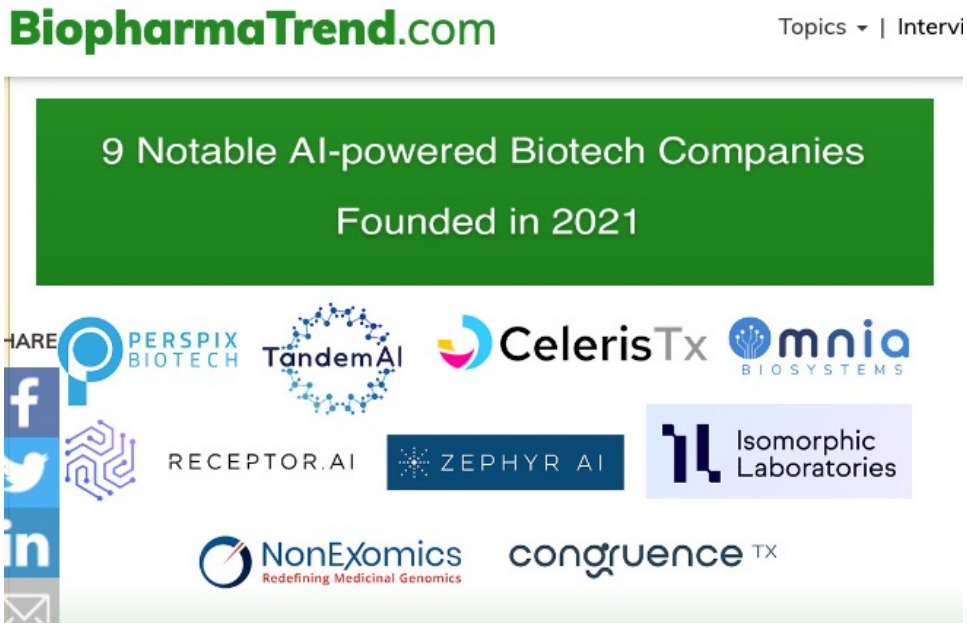
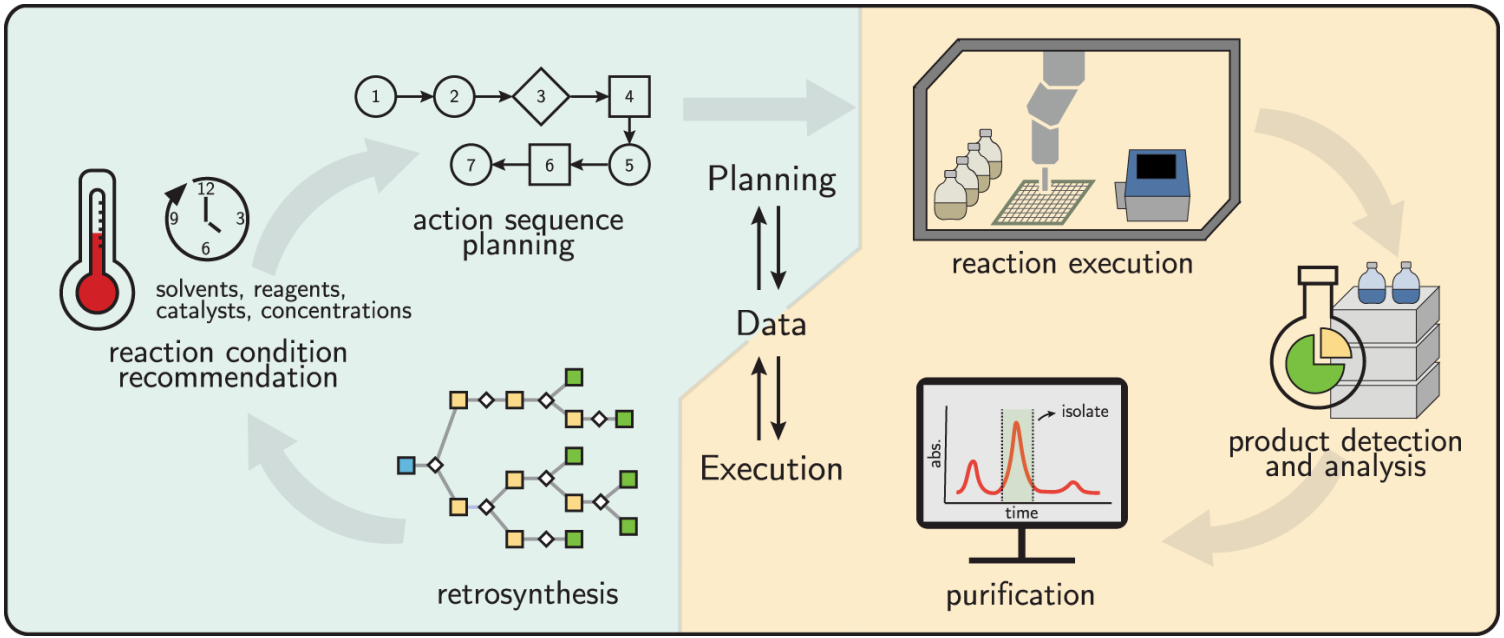


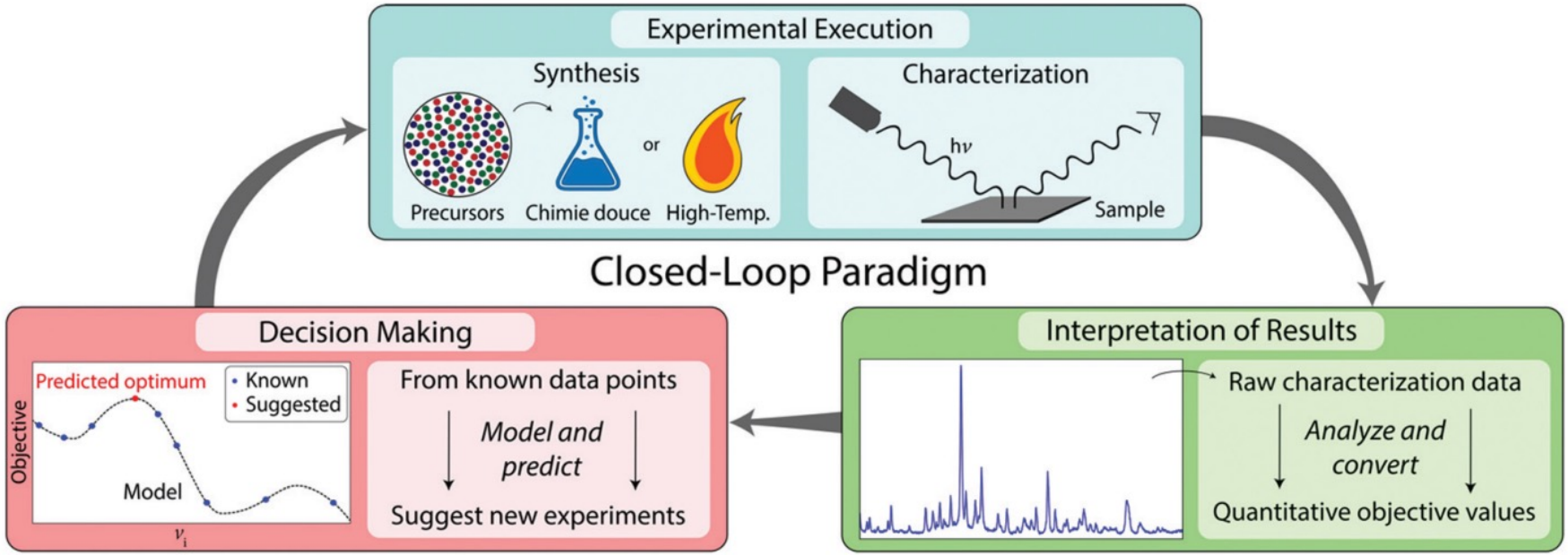
Chen, Hongming, *et al.* "The rise of deep learning in drug discovery." *Drug Discovery Today* (2018).

ML in Computational Molecular Sciences



Gao, Raghavan, Coley. "Autonomous platforms for data-driven organic synthesis." *Nature Communications* (2022).

ML in Computational Molecular Sciences



Szymanski et al. "Toward autonomous design and synthesis of novel inorganic materials." *Materials Horizons* (2021).

What is the objective with ML?

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ML helps us make sense of data more quickly

Predicting outcomes of chemical reactions:

1) Use our intuition (or collective intuition)

2) w/ ML = use trained model

3) success = trained model better than my intuition

Defining some basic terminology

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prediction = model(features)

observations = [(features, outcome), (features, outcome)...

Model learns to anticipate outcome based on the changes to features

Success is
f(1) how much good data we collect
2) how expressive our features are

Challenges of ML for science?

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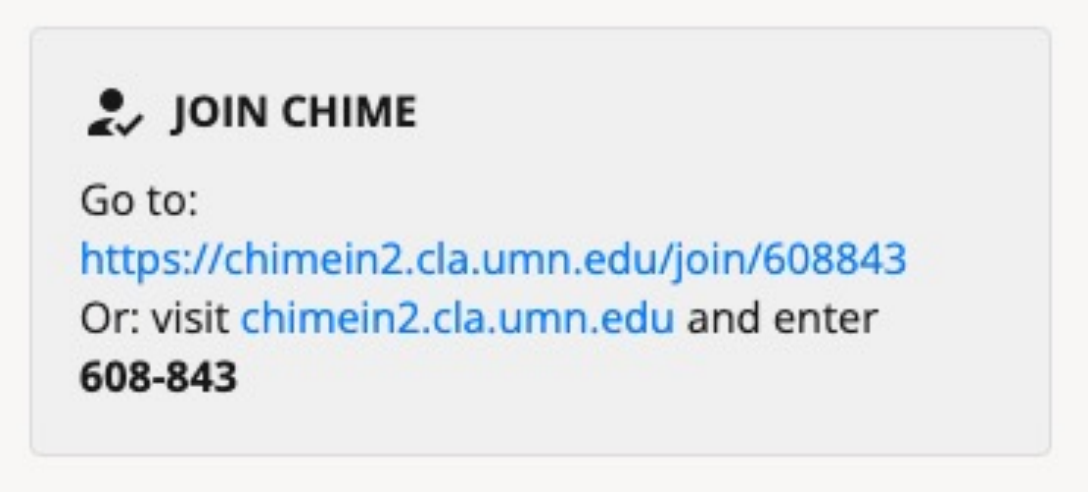
Given what you know now, discuss w/ one another some challenges of applying ML for science and engineering applications



Challenges of ML for science?

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Letter | Published: 11 September 2019

Anthropogenic biases in chemical reaction data hinder exploratory inorganic synthesis

Xiwen Jia, Allyson Lynch, Yuheng Huang, Matthew Danielson, Immaculate Lang'at, Alexander Milder, Aaron E. Ruby, Hao Wang, Sorelle A. Friedler ✉, Alexander J. Norquist ✉ & Joshua Schrier ✉

Nature **573**, 251–255 (2019) | Cite this article

7799 Accesses | **95** Citations | **68** Altmetric | Metrics

Some reactants are popular, but they aren't as good as random reactants!

Challenges of ML for science?

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Machine Learning May Sometimes Simply Capture Literature Popularity Trends: A Case Study of Heterocyclic Suzuki–Miyaura Coupling

Wiktor Beker, Rafał Roszak, Agnieszka Wołos, Nicholas H. Angello, Vandana Rathore, Martin D. Burke*, and Bartosz A. Grzybowski*

Cite this: *J. Am. Chem. Soc.* 2022, 144, 11, 4819–4827
Publication Date: March 8, 2022

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Similar story in organic chemistry…

Challenges of ML for science?

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18 Nov 2022 in Research & Technology

Cuprate superconductivity mechanism may be coming into focus

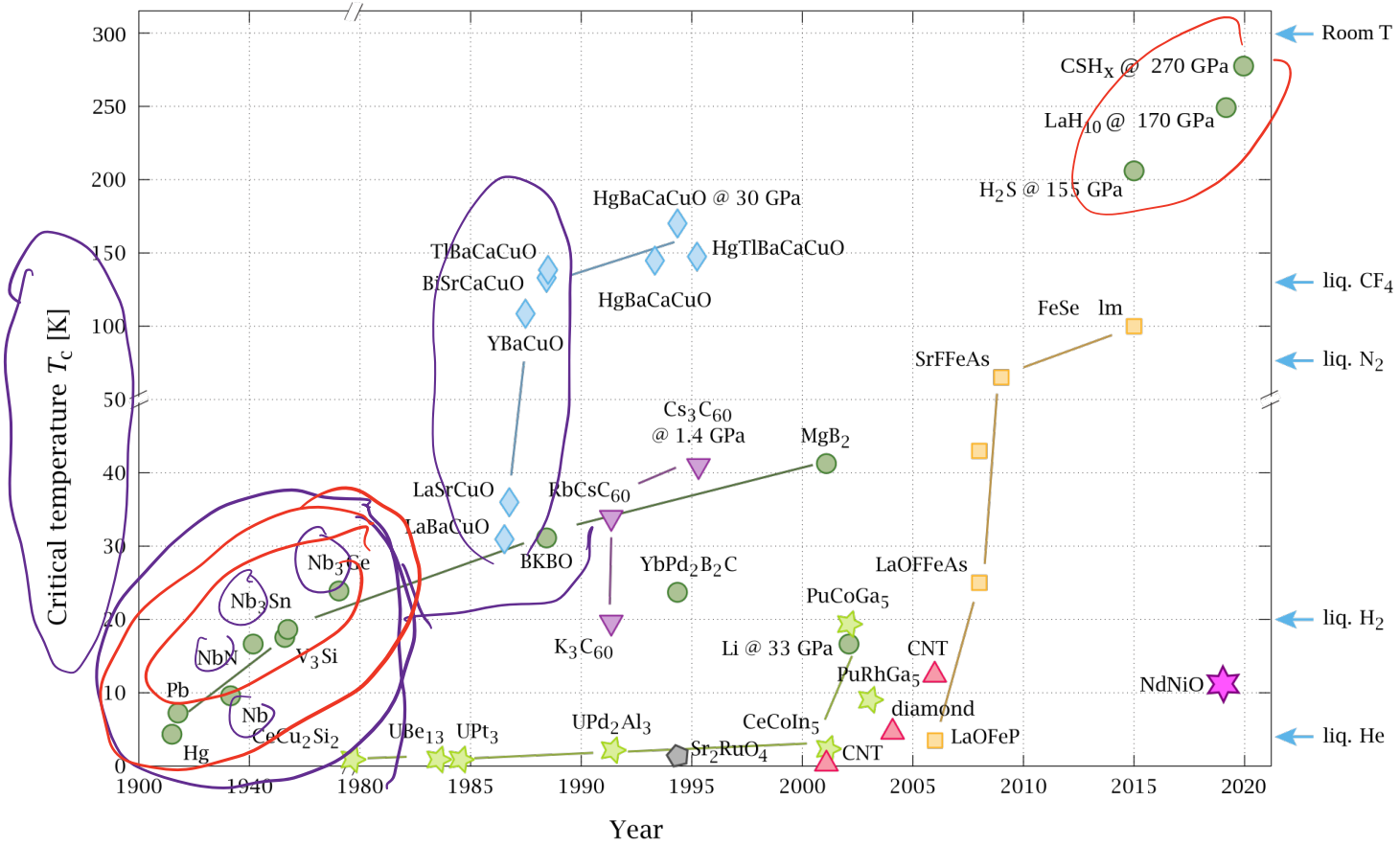
Theory and experiment have pinpointed factors that determine the magnetic attraction between electron pairs.

Daniel Garisto

Since their dramatic debut in 1986, cuprate superconductors have been some of the best-studied materials in existence. Nonetheless, many mysteries about the materials have

"Even if we are correct, in 30 years people will still say that the theory is not understood," Tremblay says.

Challenges of ML for science?



Challenges of ML for science?

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Given what you know now, discuss w/ one another some challenges of applying ML for science and engineering applications

1) Limited reliable data (hard to collect, biased, noisy)

2) Complex phenomena (hard to featurize systems)

3) Extrapolation

But it can work!!

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nature

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Article | Open Access | Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, ... Demis Hassabis + Show authors

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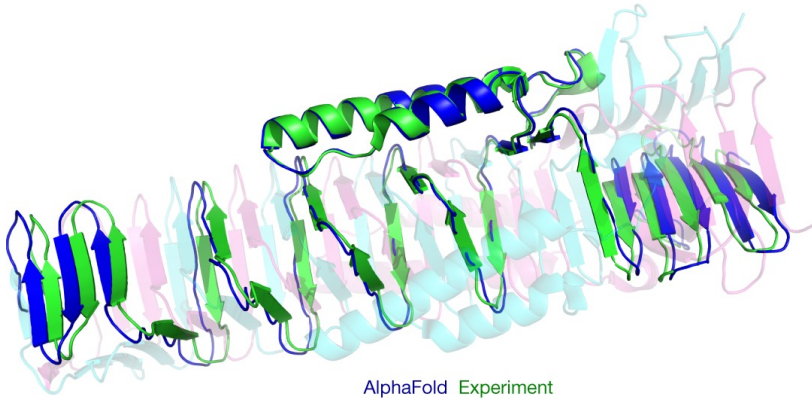

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nature

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nature › articles › article

Article | Published: 03 February 2021

Bayesian reaction optimization as a tool for chemical synthesis

Benjamin J. Shields, Jason Stevens, Jun Li, Marvin Parasram, Farhan Damani, Jesus I. Martinez Alvarado, Jacob M. Janey, Ryan P. Adams ✉ & Abigail G. Doyle ✉

Nature **590**, 89–96 (2021) | Cite this article

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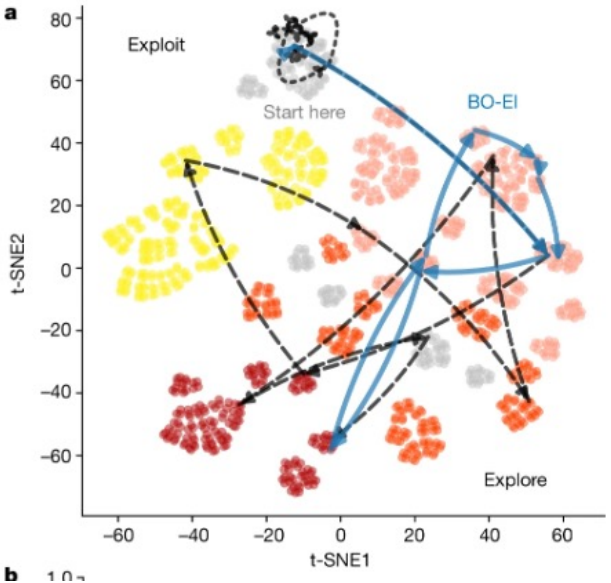

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nature › letters › article

Letter | Published: 03 July 2019

Unsupervised word embeddings capture latent knowledge from materials science literature

Vahe Tshitoyan ✉, John Dagdelen, Leigh Weston, Alexander Dunn, Ziqin Rong, Olga Kononova, Kristin A. Persson, Gerbrand Ceder ✉ & Anubhav Jain ✉

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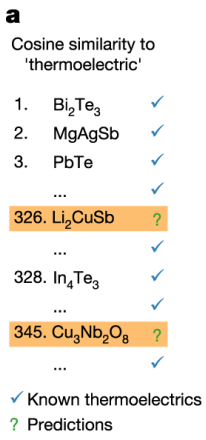

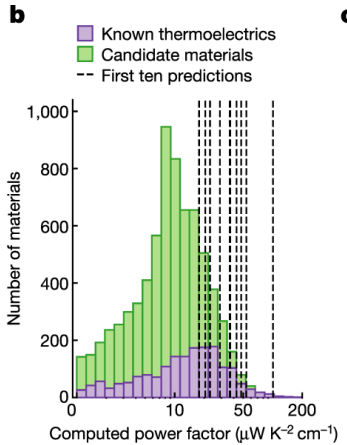

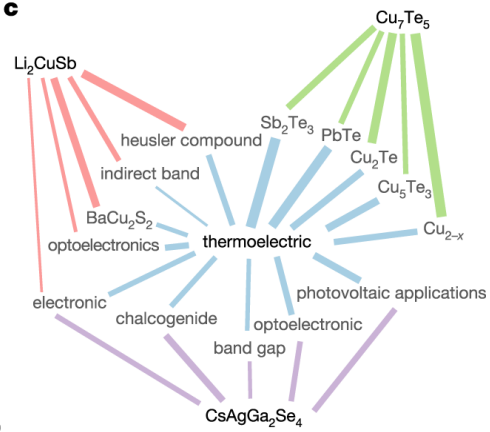

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nature energy

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Article | Published: 25 March 2019

Data-driven prediction of battery cycle life before capacity degradation

Kristen A. Severson, Peter M. Attia, Norman Jin, Nicholas Perkins, Benben Jiang, Zi Yang, Michael H. Chen, Muratahan Aykol, Patrick K. Herring, Dimitrios Fraggedakis, Martin Z. Bazant, Stephen J. Harris, William C. Chueh ✉ & Richard D. Braatz ✉

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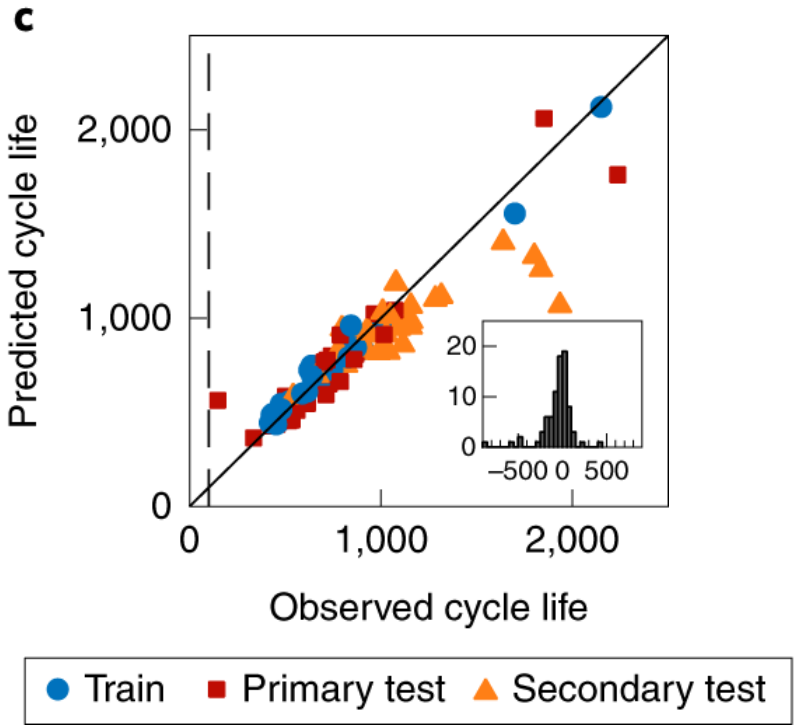

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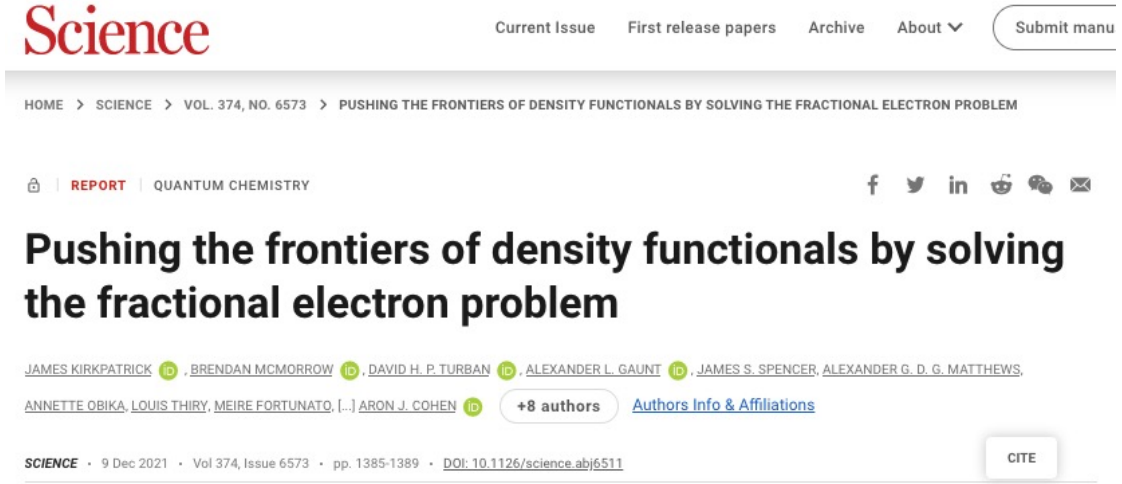

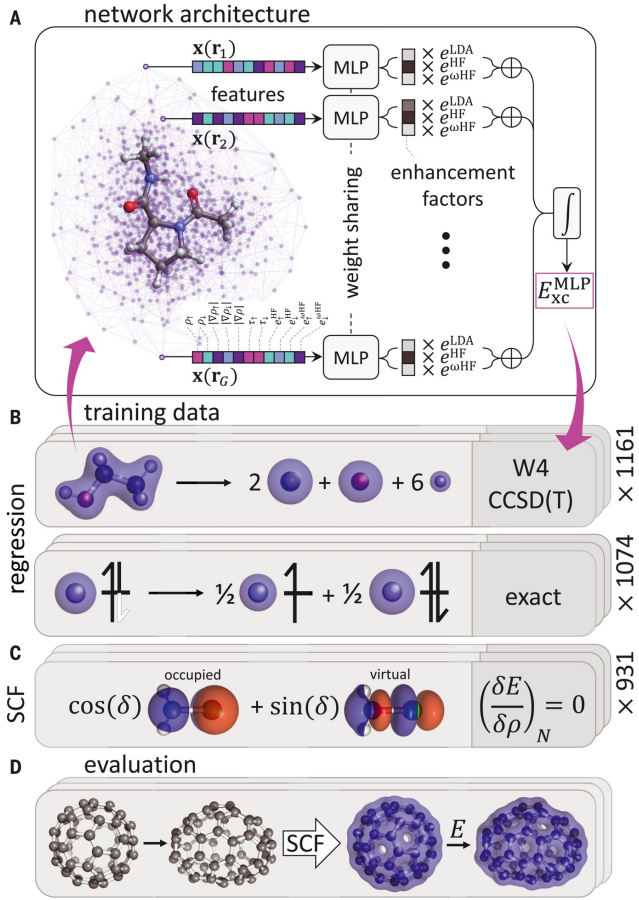

Machine learning interest on the rise!

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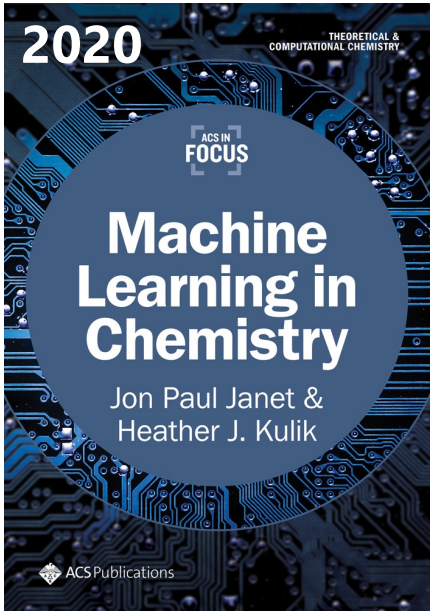

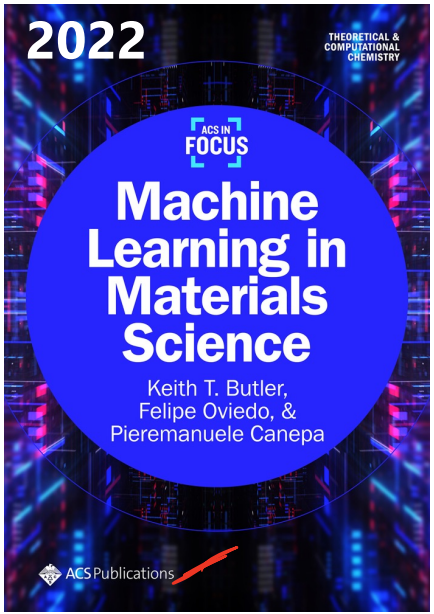

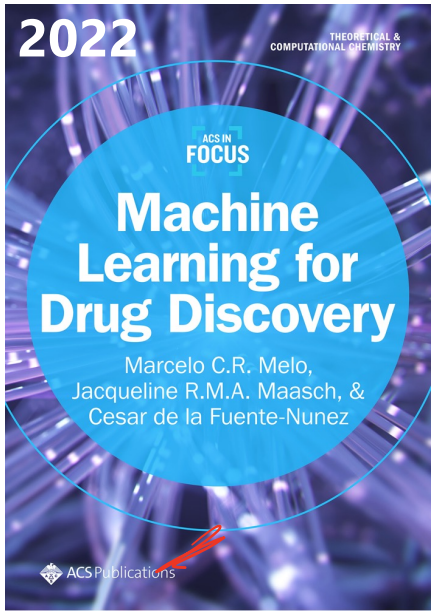

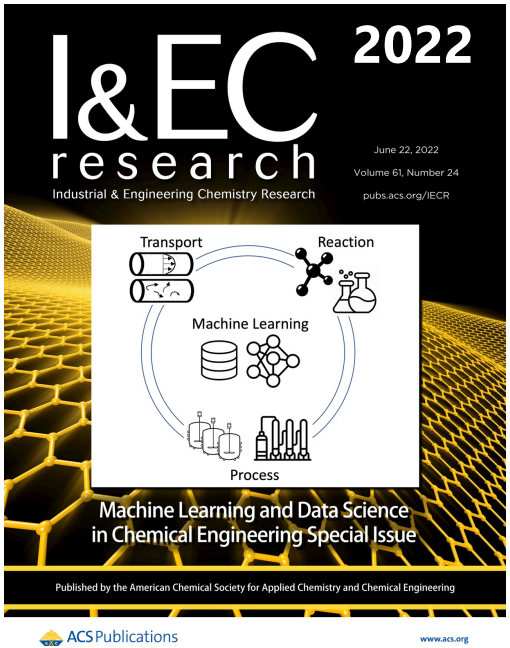

You do not need a CS degree to make meaningful contributions with ML!