



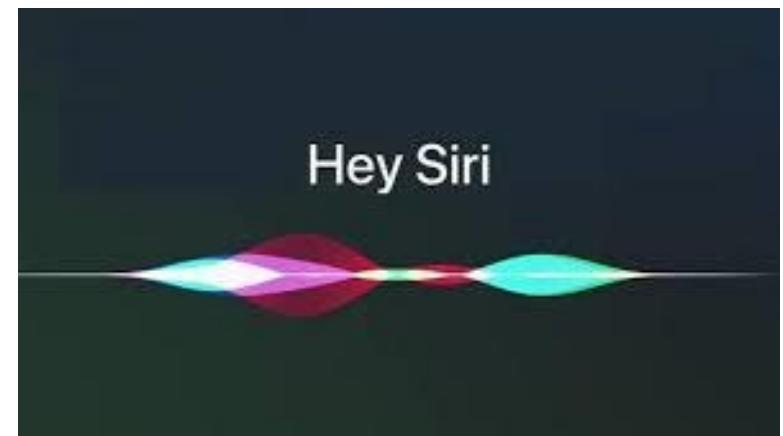
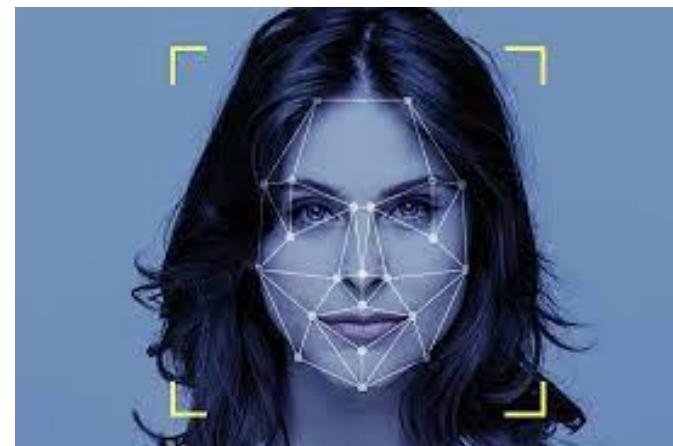
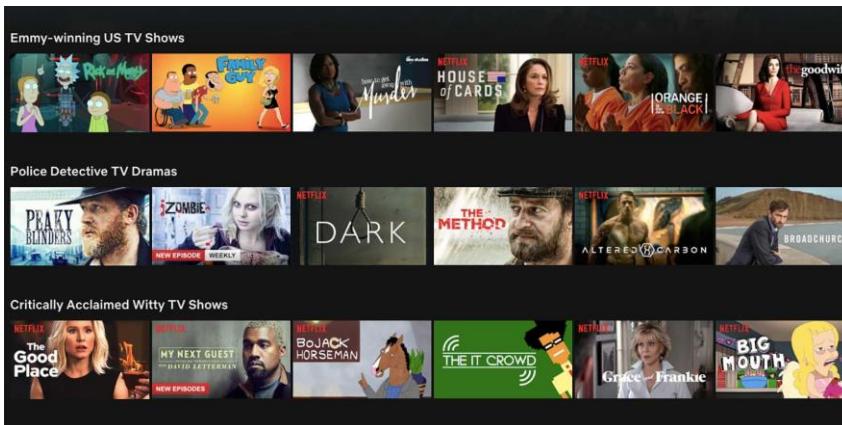
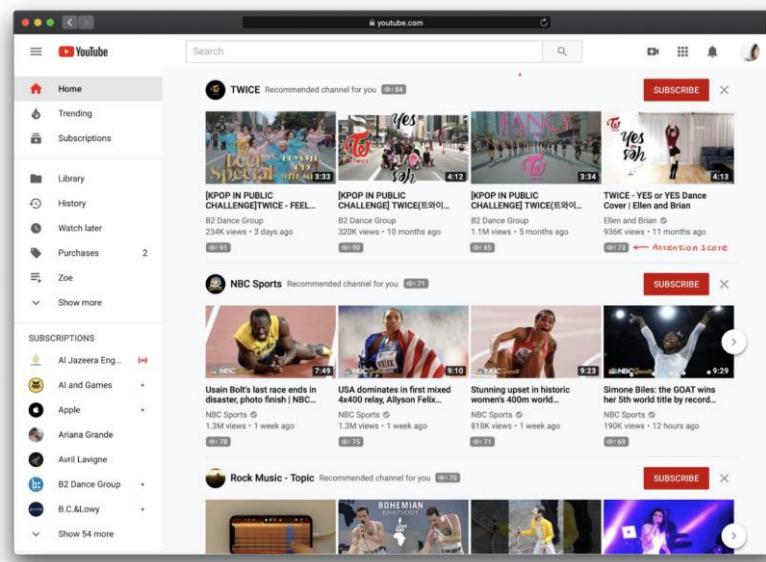
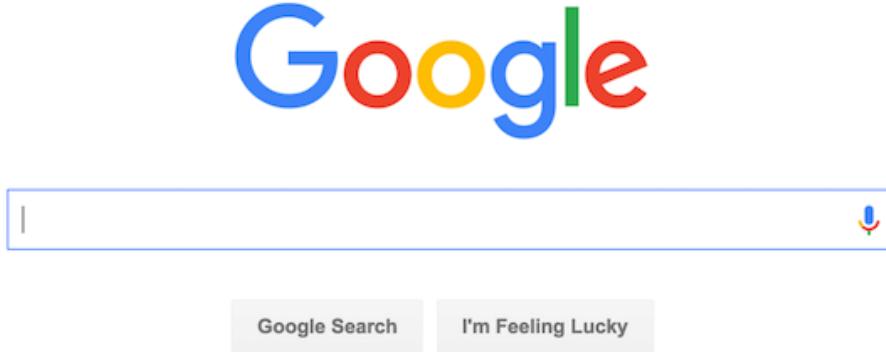
Korea Institute of Energy Technology

Artificial Intelligence

Geun Ho Gu

2024-02-25

Artificial Intelligence is everywhere



Tesla self driving



Stable Diffusion

Turtle Bug



Ulysses and the Trojan Horse Selfie



Stable Diffusion

Knight cat



rainy neon cyberpunk mega city, skyscraper, cars, people





How promising is the implementation of machine learning in materials research? Has machine learning really made innovations?



The implementation of machine learning in materials research has the potential to be highly promising and to drive significant innovations in the field. Machine learning is a type of artificial intelligence that involves training algorithms to recognize patterns in data, and it can be used to analyze and interpret complex data sets in materials research.



There are several examples of how machine learning has already made significant contributions to the field of materials science. For example:

1. Materials discovery: Machine learning algorithms can be used to analyze large amounts of data to identify new materials with desirable properties, such as increased strength, durability, and conductivity.
2. Materials characterization: Machine learning can be used to automatically analyze data from materials characterization techniques, such as X-ray diffraction or electron microscopy, to determine the structure and composition of materials.
3. Materials simulation: Machine learning algorithms can be used to accelerate and optimize materials simulations, allowing for the prediction of properties and behavior of materials in different conditions.
4. Materials design: Machine learning can be used to optimize the design of materials with specific properties, such as increased strength, improved thermal stability, or enhanced electrical conductivity.

Overall, the implementation of machine learning in materials research has the potential to significantly advance the field and drive the discovery and development of new materials with a wide range of applications. It's important to note that machine learning is still a relatively new tool in materials science, and its full potential has yet to be realized.

Regenerate response

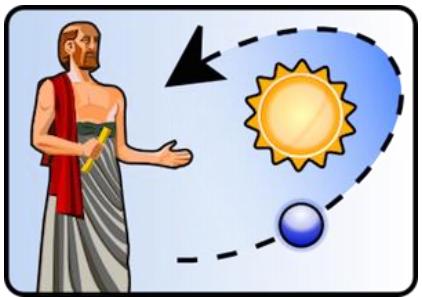
OpenAI Sora 2/18/2024



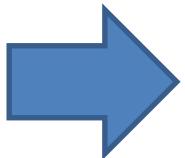
Digital Chemistry

Evolution of Science

Observation



Aristarchus



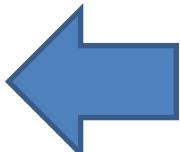
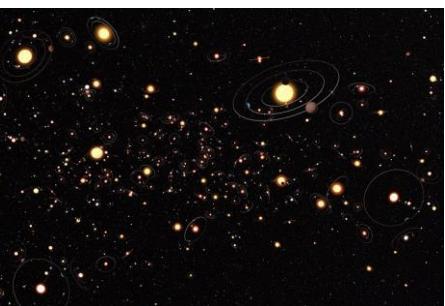
Rules



Kepler



Theory



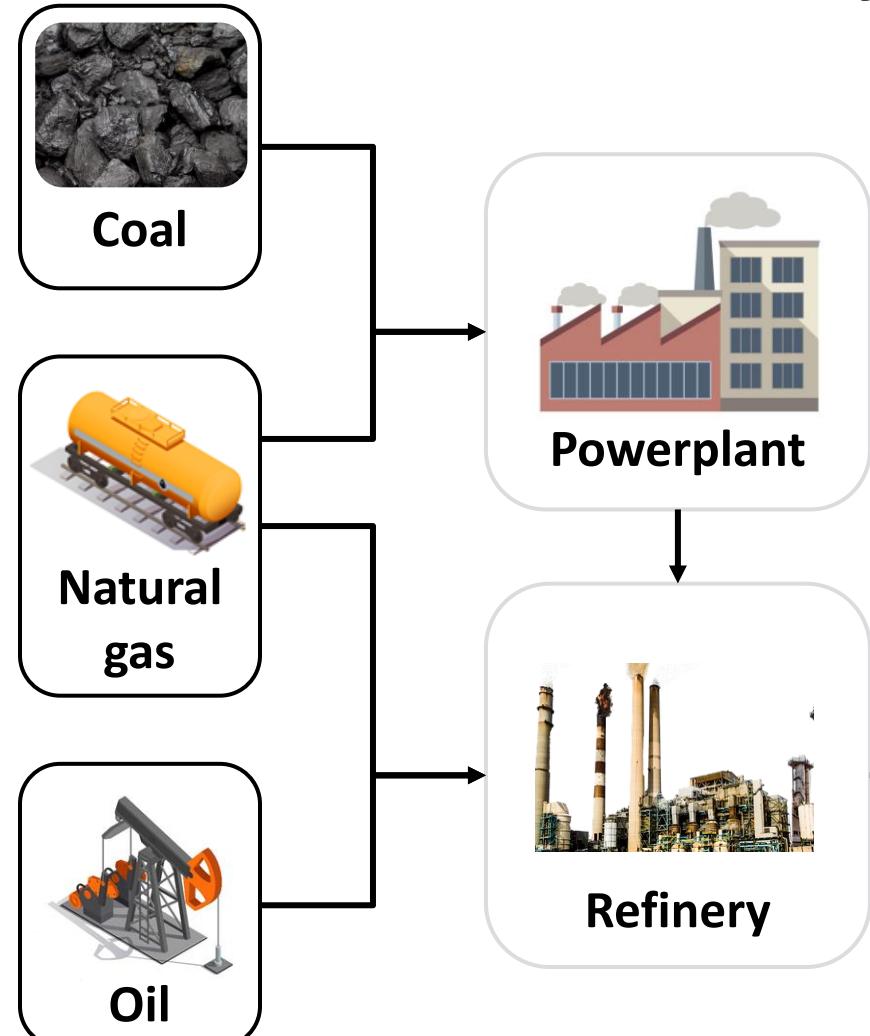
Data Science
Discovery of new planets
from planets' motion



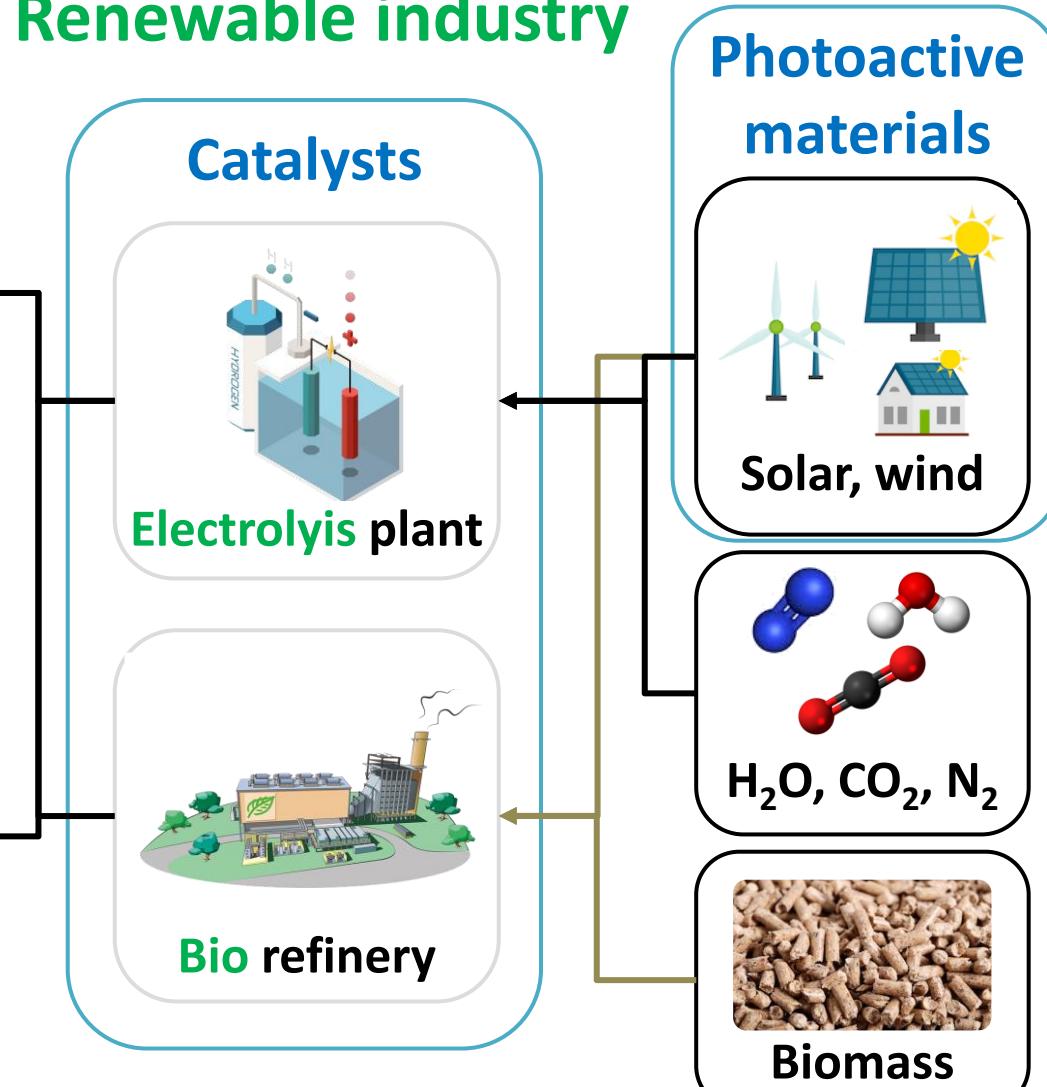
Isaac Newton

Renewable Energy Society Portfolio

Fossil industry

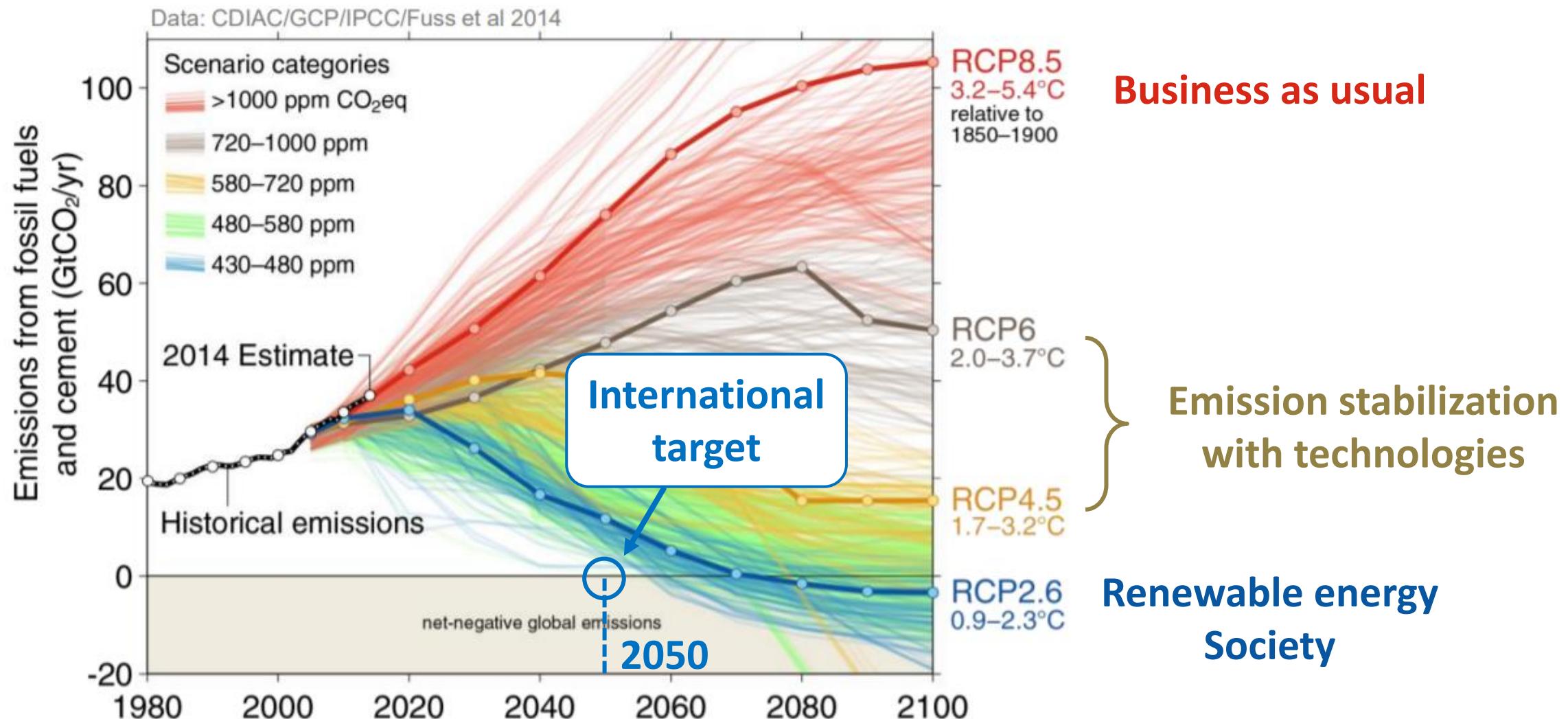


Renewable industry



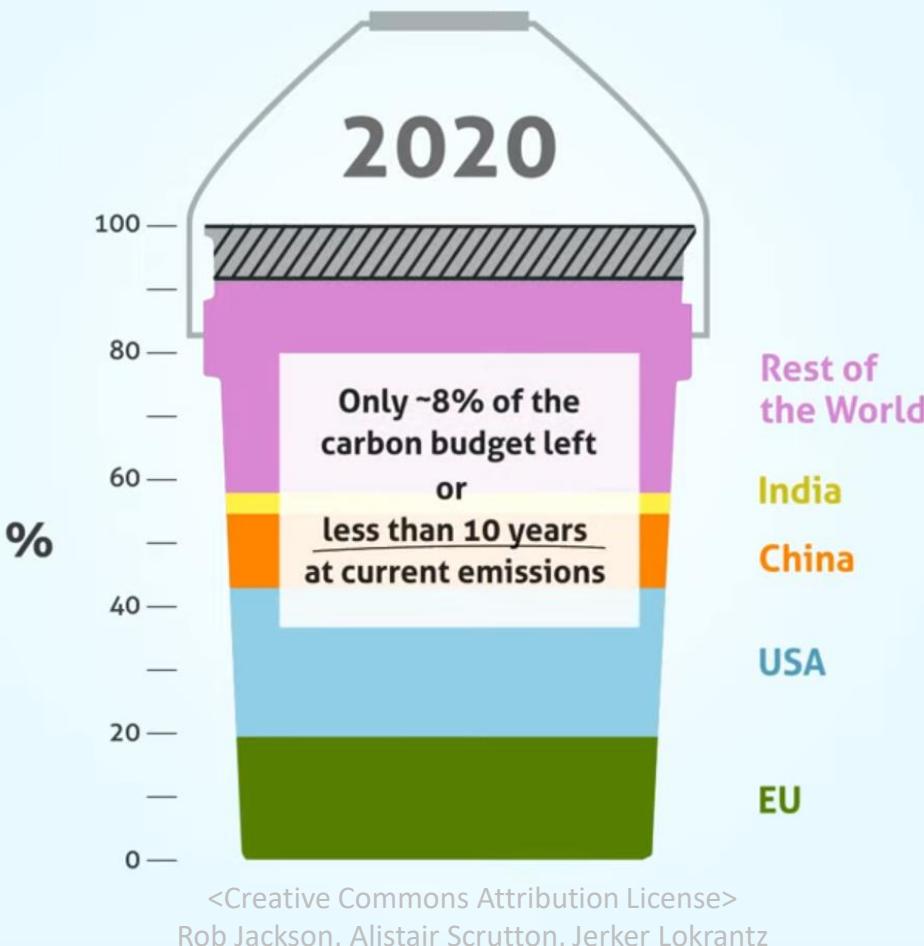
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Innovation Needed to Cut Emissions



Carbon Budget and Need for Accelerated Research

The carbon budget for 1.5 degrees



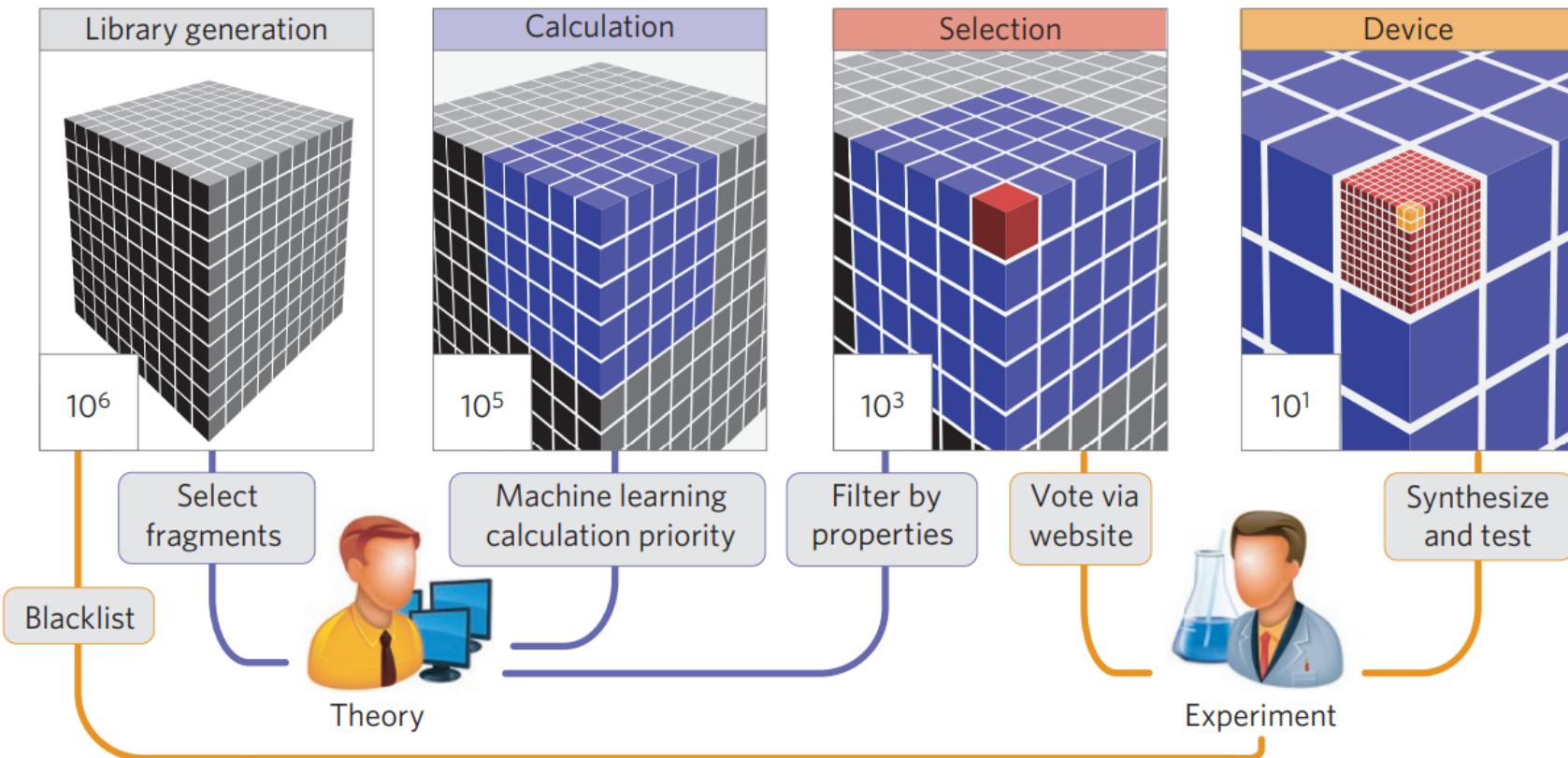
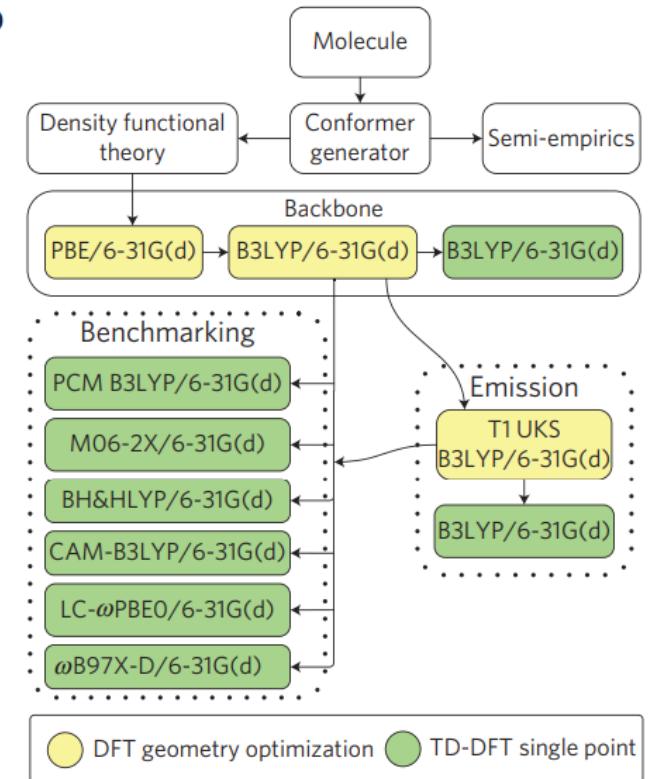
Challenges

- The 1.5°C scenario carbon budget runs out in 6 years
- The deployment of new technology takes 10-20 years

We need to accelerate research!

Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach

Rafael Gómez-Bombarelli¹, Jorge Aguilera-Iparraguirre¹, Timothy D. Hirzel¹, David Duvenaud², Dougal Maclaurin², Martin A. Blood-Forsythe¹, Hyun Sik Chae³, Markus Einzinger⁴, Dong-Gwang Ha⁵, Tony Wu⁴, Georgios Markopoulos⁶, Soonok Jeon⁷, Hosuk Kang⁷, Hiroshi Miyazaki⁷, Masaki Numata⁷, Sunghan Kim⁷, Wenliang Huang⁶, Seong Ik Hong³, Marc Baldo⁴, Ryan P. Adams² and Alán Aspuru-Guzik^{1*}

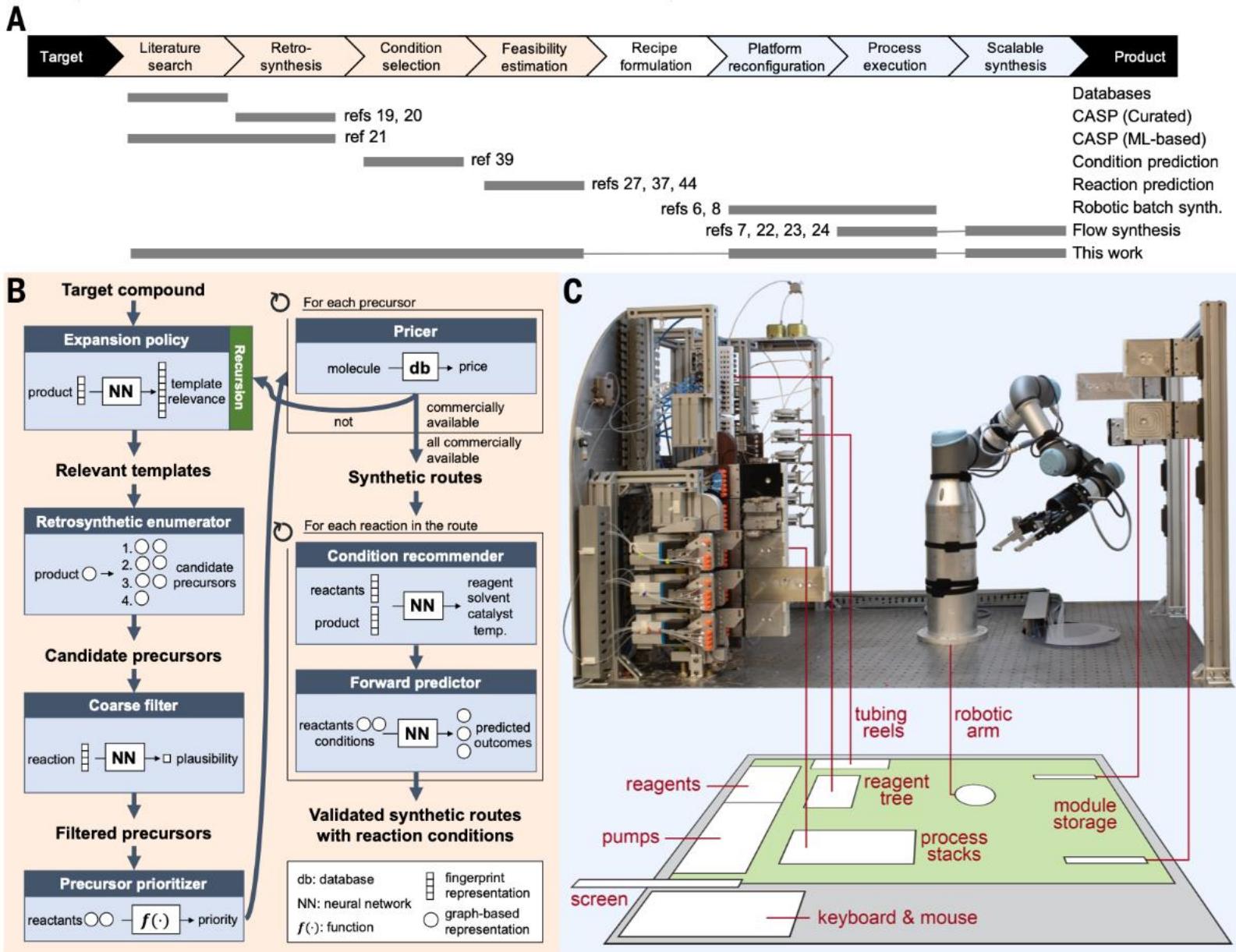
a**b**

RESEARCH ARTICLE SUMMARY

ORGANIC CHEMISTRY

A robotic platform for flow synthesis of organic compounds informed by AI planning

Connor W. Coley*, **Dale A. Thomas III***, **Justin A. M. Lummiss***, **Jonathan N. Jaworski**,
Christopher P. Breen, **Victor Schultz**, **Travis Hart**, **Joshua S. Fishman**, **Luke Rogers**,
Hanyu Gao, **Robert W. Hicklin**, **Pieter P. Plehiers**, **Joshua Byington**, **John S. Piotti**,
William H. Green, **A. John Hart**, **Timothy F. Jamison†**, **Klavs F. Jensen†**

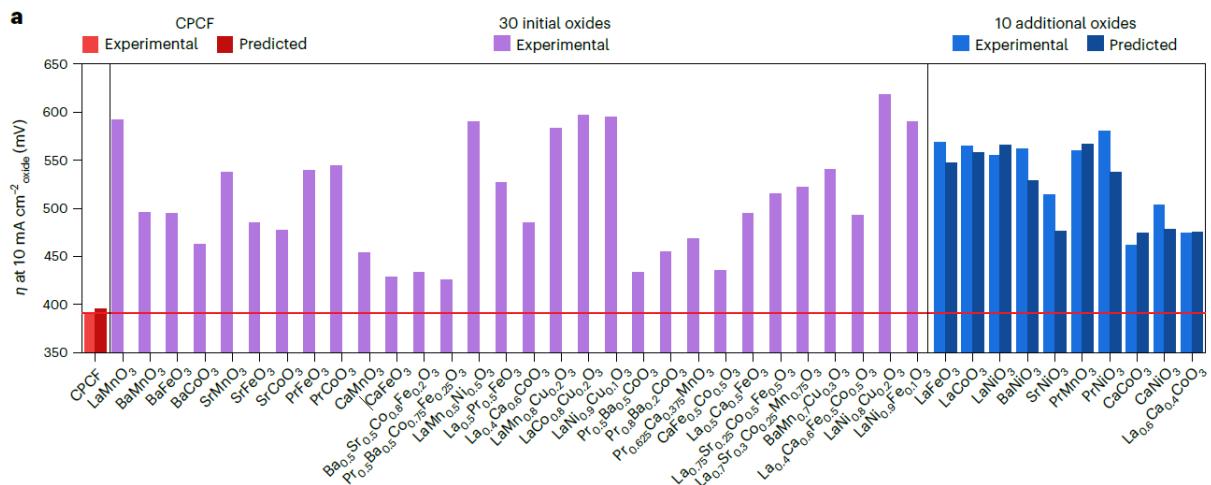
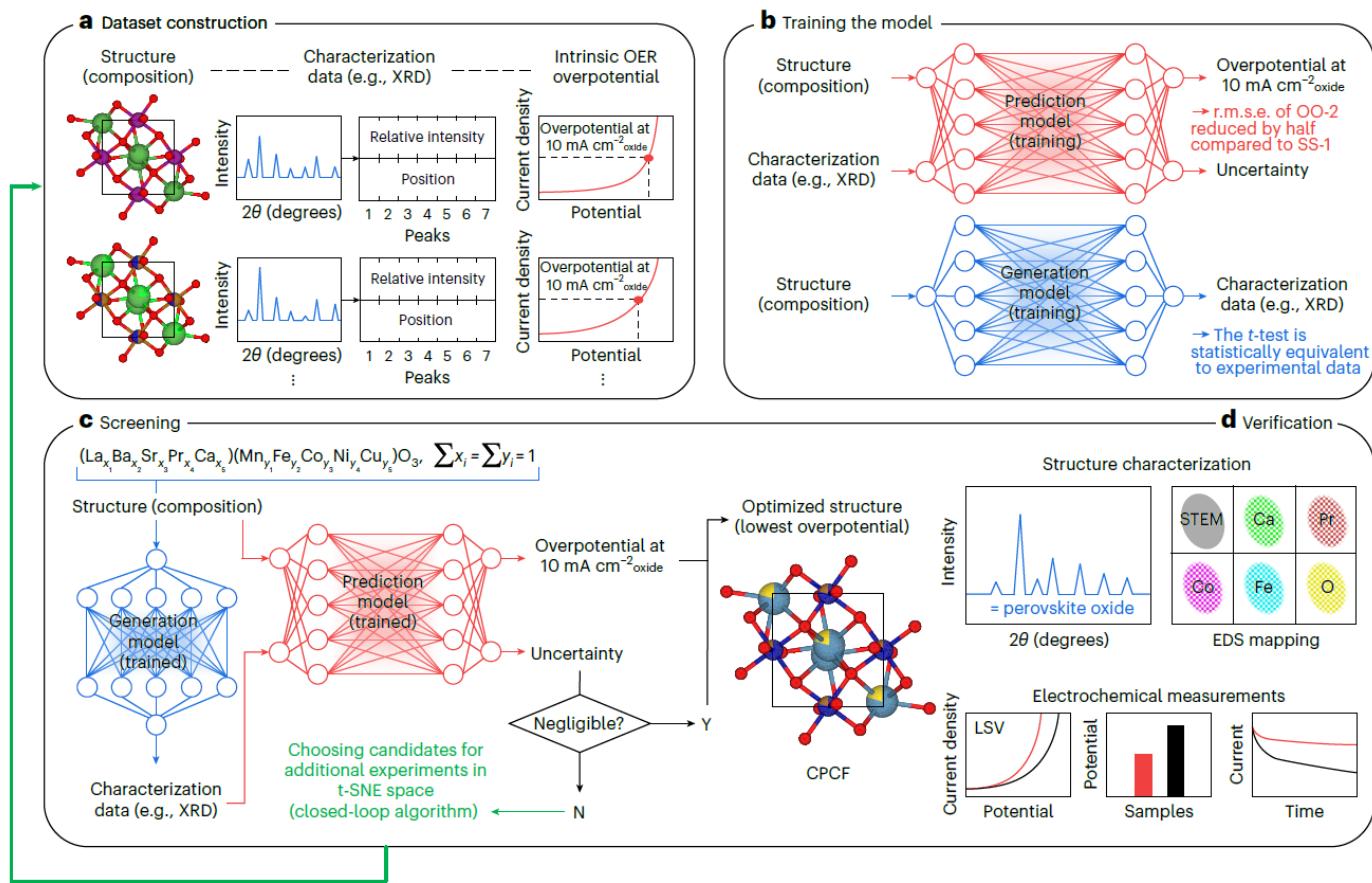


Active learning guides discovery of a champion four-metal perovskite oxide for oxygen evolution electrocatalysis

Received: 24 November 2022

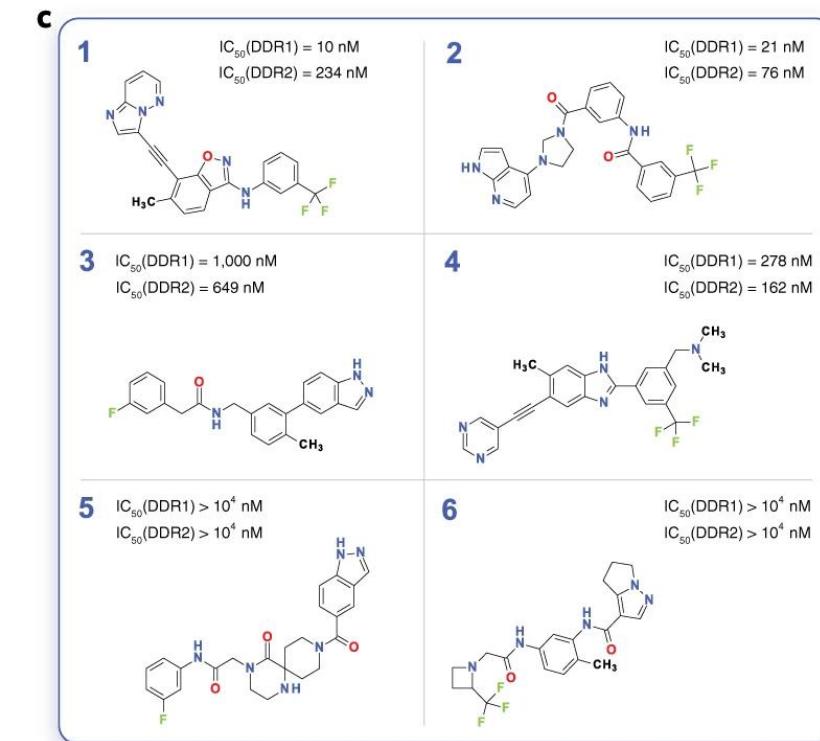
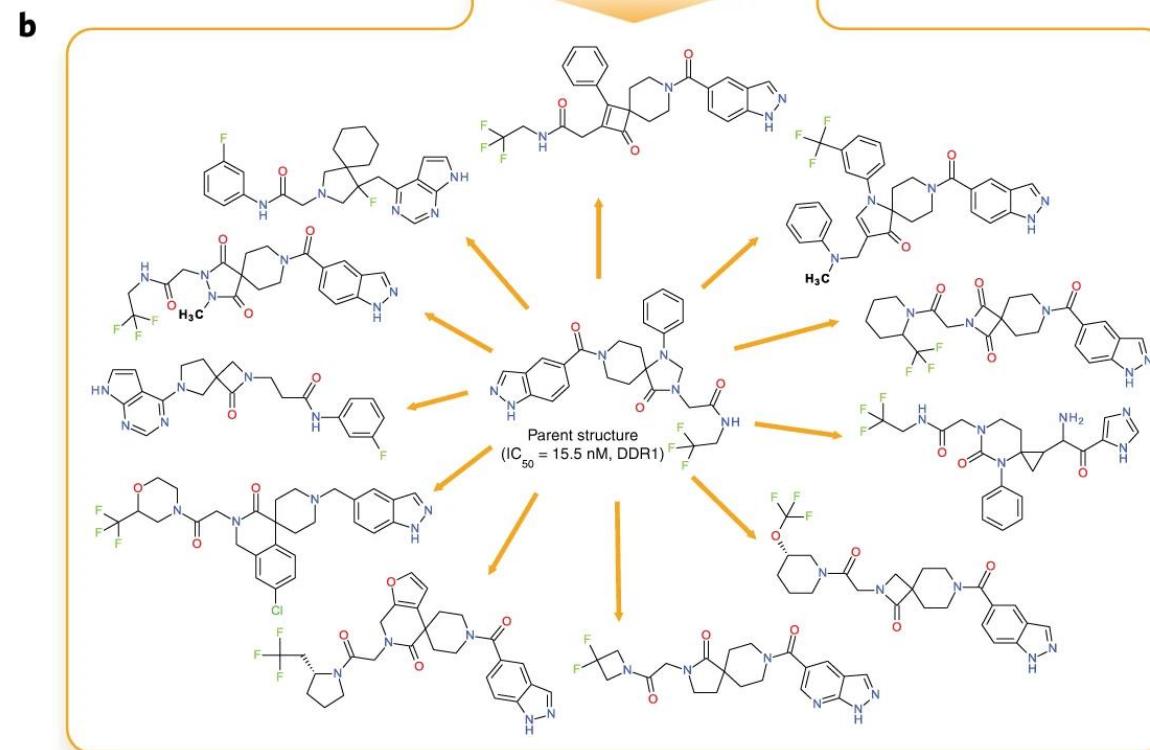
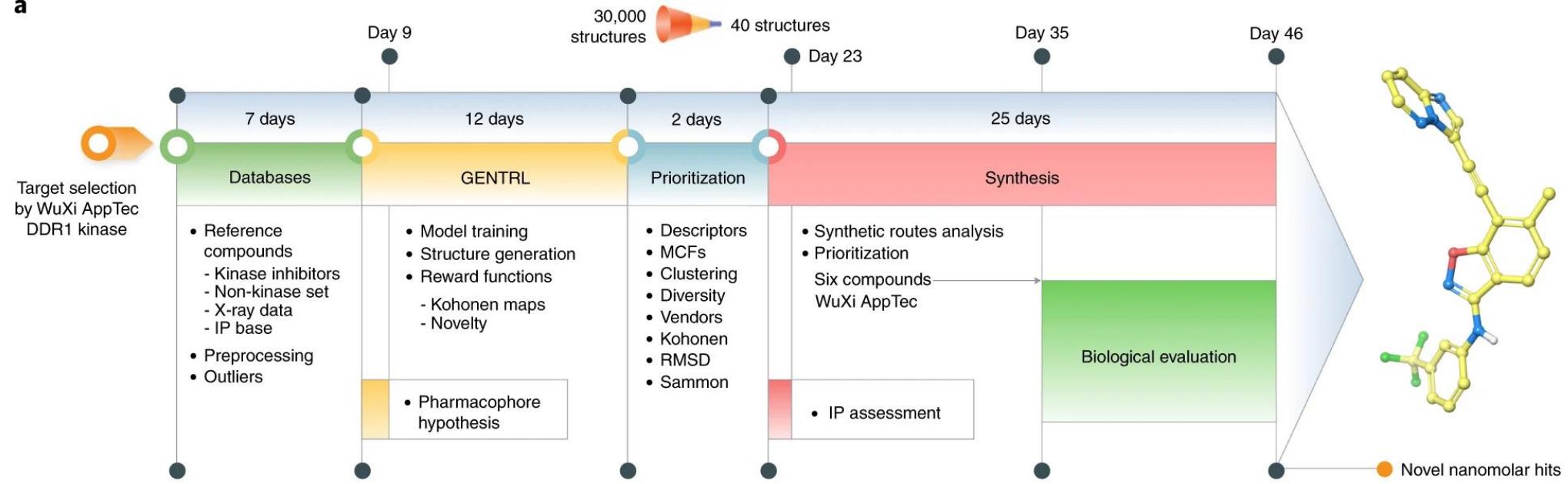
Accepted: 2 October 2023

Junseok Moon^{1,2}, Wiktor Beker^{3,4}, Marta Siek^{1,2}, Jiheon Kim^{1,2},
Hyeon Seok Lee^{1,2}, Taeghwan Hyeon^{1,2✉} & Bartosz A. Grzybowski^{1,2✉}



Deep learning enables rapid identification of potent DDR1 kinase inhibitors

Alex Zhavoronkov^{1*}, Yan A. Ivanenkov¹, Alex Aliper¹, Mark S. Veselov¹, Vladimir A. Aladinskiy¹, Anastasiya V. Aladinskaya¹, Victor A. Terentiev¹, Daniil A. Polykovskiy¹, Maksim D. Kuznetsov¹, Arip Asadulaev¹, Yury Volkov¹, Artem Zholus¹, Rim R. Shayakhmetov¹, Alexander Zhebrak¹, Lidiya I. Minaeva¹, Bogdan A. Zagribelnyy¹, Lennart H. Lee^{1,2}, Richard Soll², David Madge², Li Xing², Tao Guo^{1,2} and Alán Aspuru-Guzik^{3,4,5,6}



Article

Highly accurate protein structure prediction with AlphaFold

<https://doi.org/10.1038/s41586-021-03819-2>

Received: 11 May 2021

Accepted: 12 July 2021

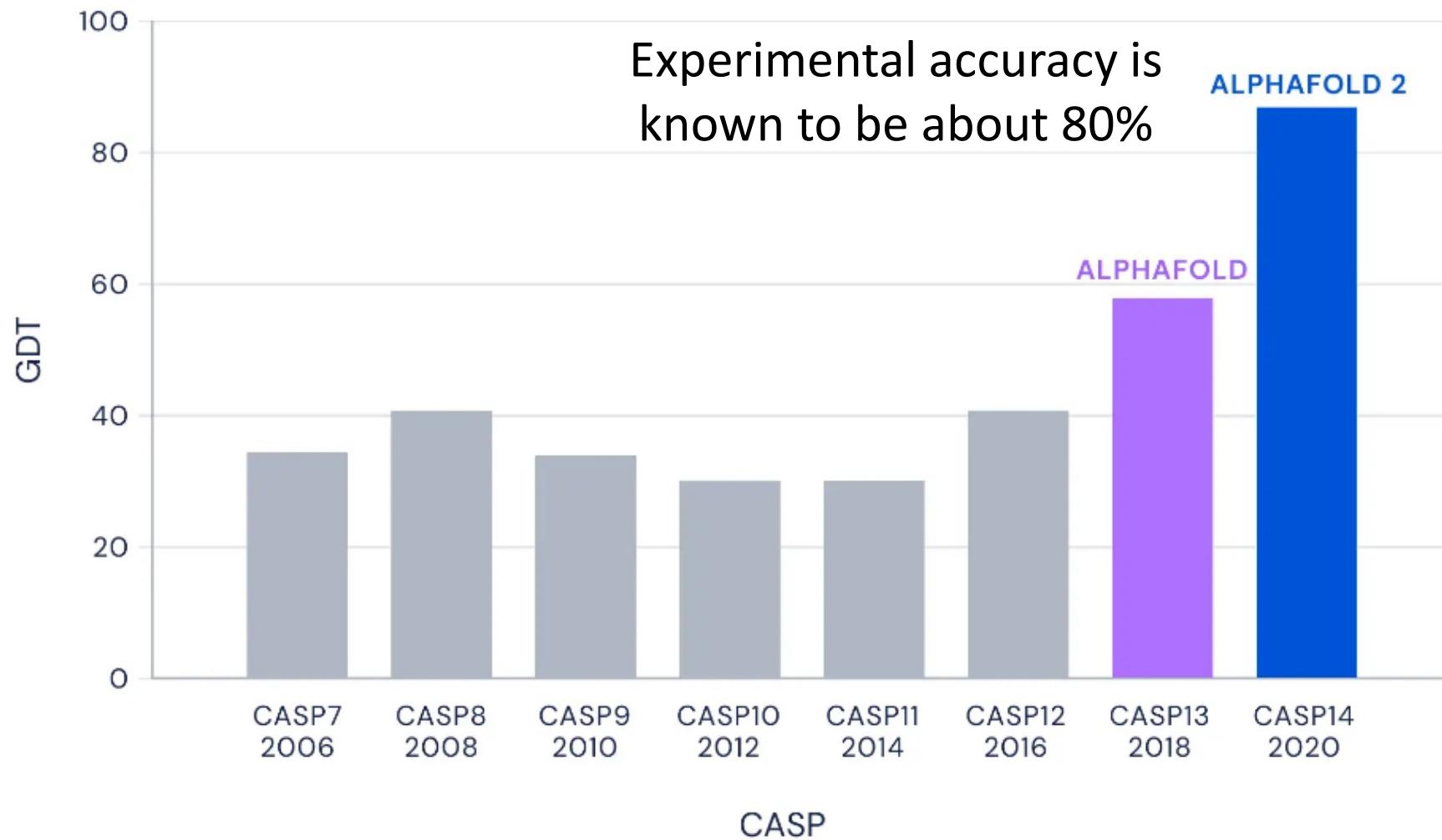
Published online: 15 July 2021

Open access

 Check for updates

John Jumper^{1,4}✉, Richard Evans^{1,4}, Alexander Pritzel^{1,4}, Tim Green^{1,4}, Michael Figurnov^{1,4}, Olaf Ronneberger^{1,4}, Kathryn Tunyasuvunakool^{1,4}, Russ Bates^{1,4}, Augustin Žídek^{1,4}, Anna Potapenko^{1,4}, Alex Bridgland^{1,4}, Clemens Meyer^{1,4}, Simon A. A. Kohl^{1,4}, Andrew J. Ballard^{1,4}, Andrew Cowie^{1,4}, Bernardino Romera-Paredes^{1,4}, Stanislav Nikolov^{1,4}, Rishabh Jain^{1,4}, Jonas Adler¹, Trevor Back¹, Stig Petersen¹, David Reiman¹, Ellen Clancy¹, Michał Zieliński¹, Martin Steinegger^{2,3}, Michałina Pacholska¹, Tamas Berghammer¹, Sebastian Bodenstein¹, David Silver¹, Oriol Vinyals¹, Andrew W. Senior¹, Koray Kavukcuoglu¹, Pushmeet Kohli¹ & Demis Hassabis^{1,4}✉

Median Free-Modelling Accuracy



AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism

BETA

Search

Examples:

Free fatty acid receptor 2

At1g58602

Q5VSL9

E. coli

Help: [AlphaFold DB search help](#)

Feedback on structure: [Contact DeepMind](#)

**Over 350,000 protein structures, including 20,000
proteins expressed in the human body**

Article

Accelerated discovery of CO₂ electrocatalysts using active machine learning

<https://doi.org/10.1038/s41586-020-2242-8>

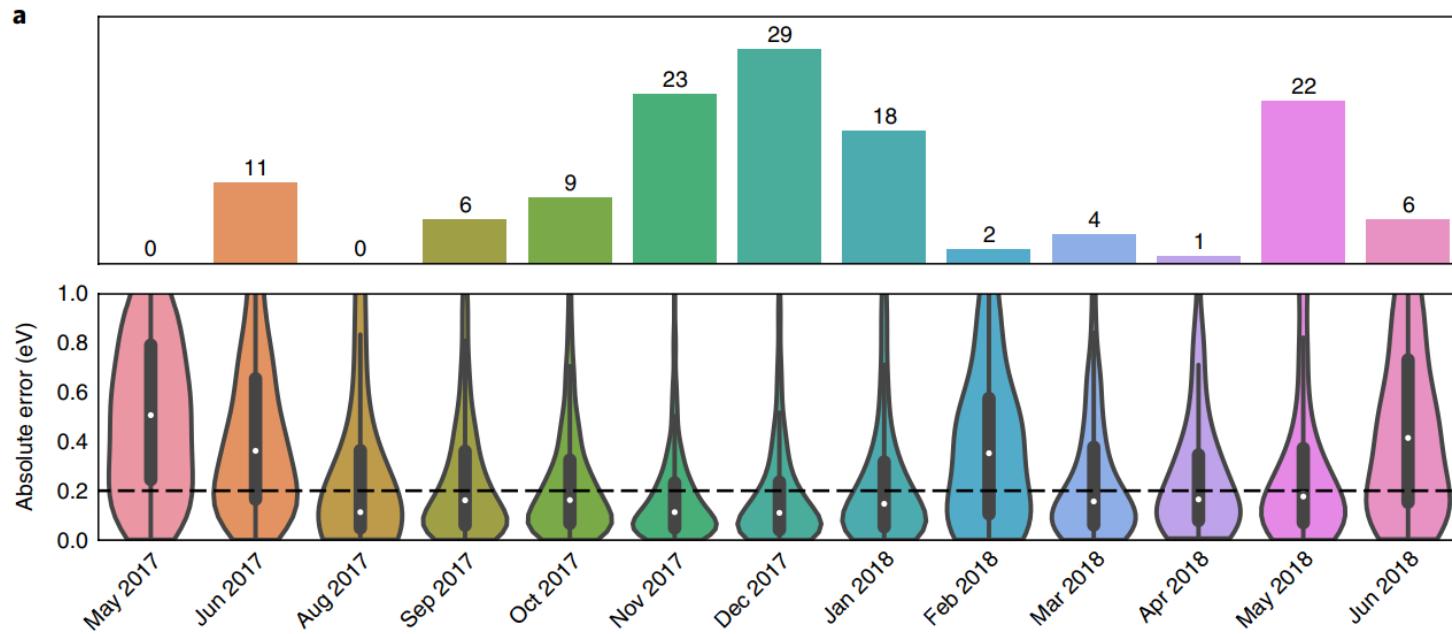
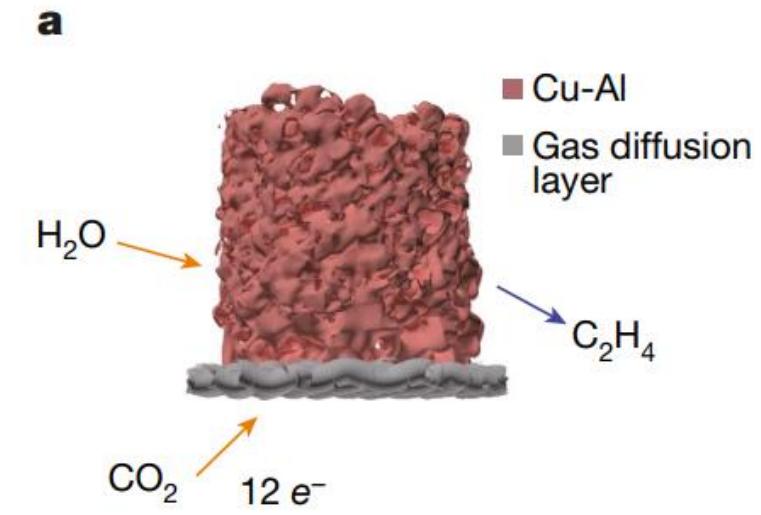
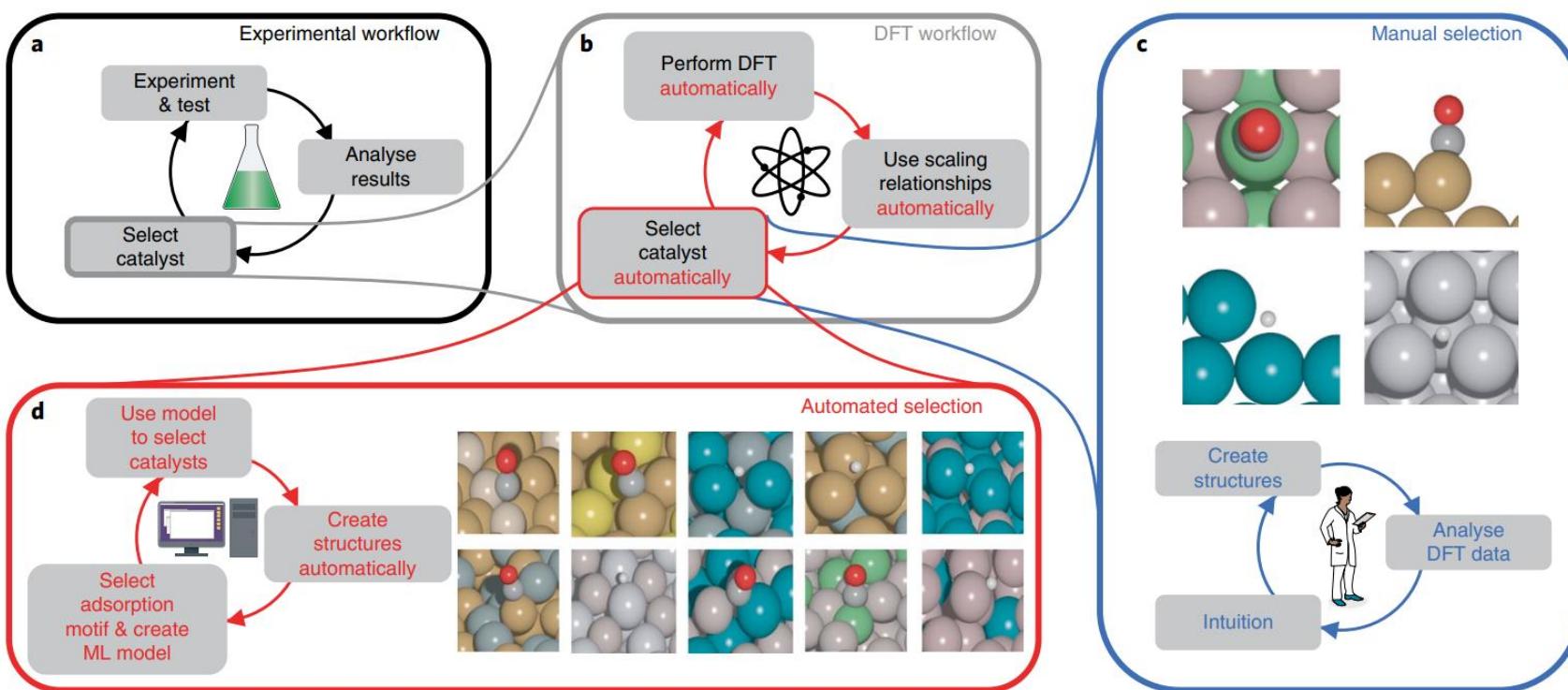
Received: 14 April 2018

Accepted: 13 March 2020

Published online: 13 May 2020

 Check for updates

Miao Zhong^{1,2,9}, Kevin Tran^{3,9}, Yimeng Min^{1,9}, Chuanhao Wang^{1,9}, Ziyun Wang¹, Cao-Thang Dinh¹, Phil De Luna^{4,8}, Zongqian Yu³, Armin Sedighian Rasouli¹, Peter Brodersen⁵, Song Sun⁶, Oleksandr Voznyy¹, Chih-Shan Tan¹, Mikhail Askerka¹, Fanglin Che¹, Min Liu¹, Ali Seifitokaldani¹, Yuanjie Pang¹, Shen-Chuan Lo⁷, Alexander Ip¹, Zachary Ulissi³✉ & Edward H. Sargent¹✉



Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation

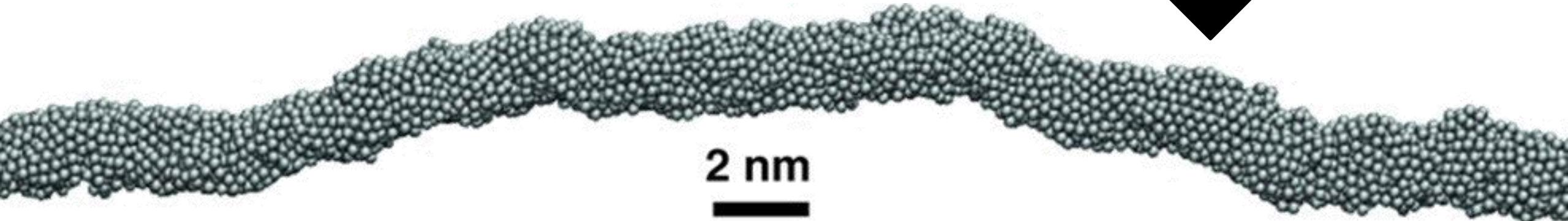
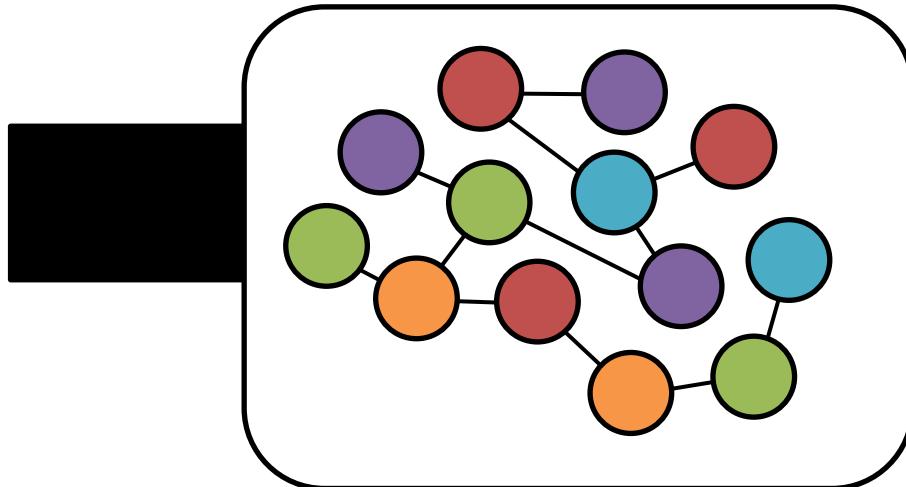
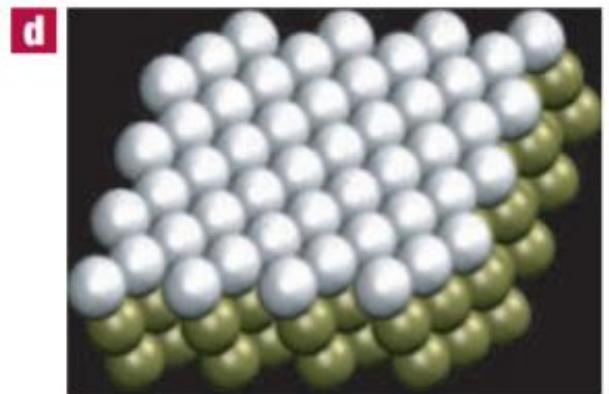
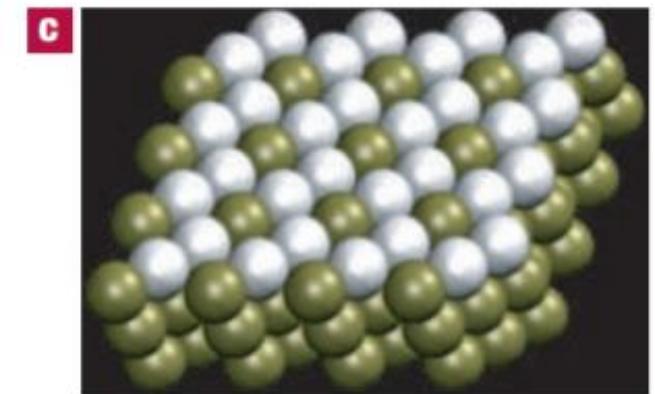
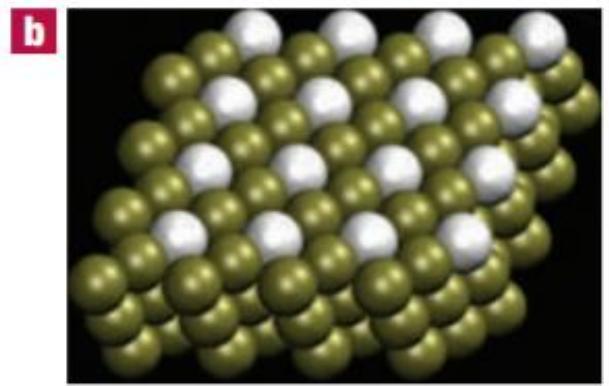
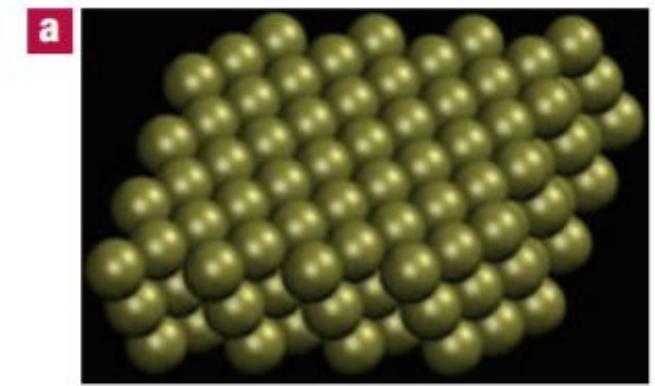
Geun Ho Gu, Juhyung Lim, Chengzhang Wan, Tao Cheng, Heting Pu, Sungwon Kim, Juhwan Noh, Changhyeok Choi, Juhwan Kim, William A. Goddard, III,* Xiangfeng Duan,* and Yousung Jung*



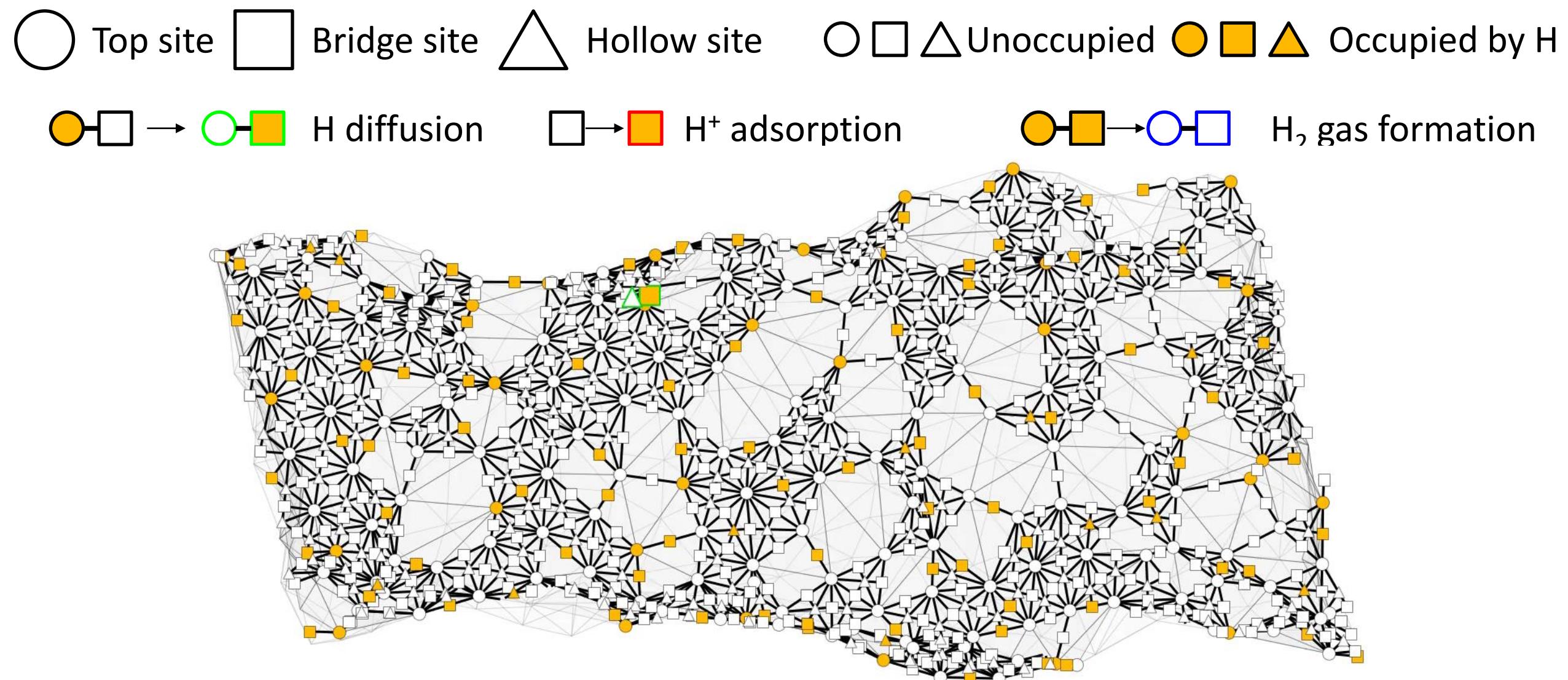
Cite This: *J. Am. Chem. Soc.* 2021, 143, 5355–5363



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Kinetic Monte Carlo Simulation



Structure-Based Synthesizability Prediction of Crystals Using Partially Supervised Learning

Jidon Jang,[†] Geun Ho Gu,[†] Juhwan Noh, Juhwan Kim, and Yousung Jung*

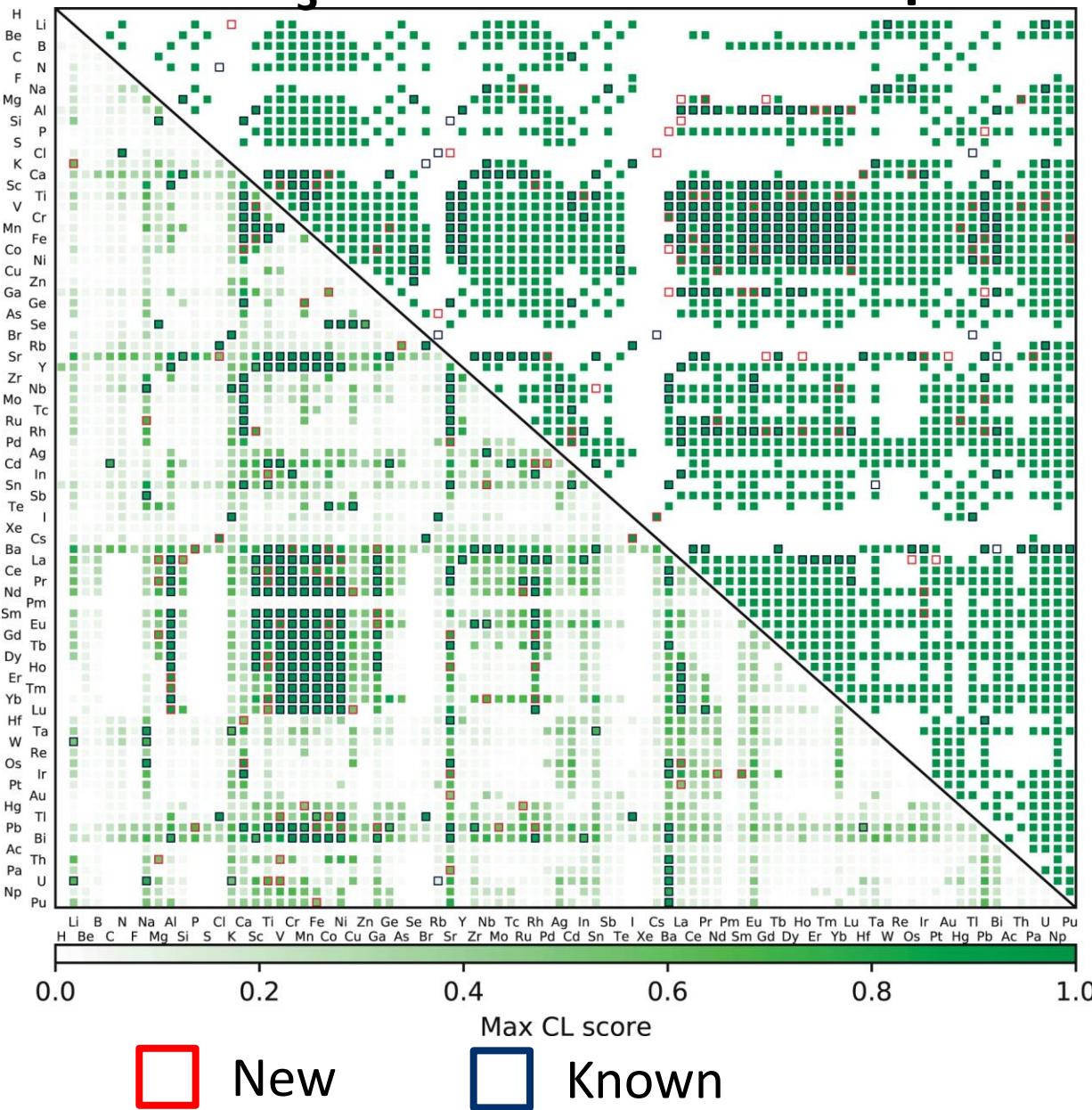


Cite This: *J. Am. Chem. Soc.* 2020, 142, 18836–18843



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ABO_3 Perovskite Oxide Map



Discovery of New Halide Perovskite

Table 1. Synthesizable halide perovskites with calculated bandgap in-between 0.7 and 2.0 eV for photovoltaics applications.

ABC_3	Bandgap [eV]	CL score	Energy above hull (eV/atom)
RbCoF_3	0.71	0.861	0.016
KGeBr_3	0.85	0.559	0.000
NPF_3	0.85	0.545	1.706
CsNaF_3	0.94	0.820	0.025
NaCuCl_3	1.36	0.797	0.002
RbCF_3	1.39	0.631	1.154
KGeCl_3	1.43	0.544	0.015
TlGeCl_3	1.46	0.572	0.019
CsPdF_3	1.52	0.814	0.102
RbCrF_3	1.82	0.560	0.097
RbOF_3	1.92	0.586	0.374
InGeCl_3	1.99	0.617	0.039

Flipped Learning

- All lectures are pre-recorded and will be available a week prior.
- Students will watch the lecture at home, solve problem sets before the class. Students are encouraged to work together!
- **Problem set is to be submitted online before the class.** The effort and completeness will be graded.
- During the class, students as many as the problems will be randomly selected to explain the solution to the class.
- Students will get +1 point for presenting, -1 for absence, 0 for a pass or poor effort. These points will be **the basis for the participation score.** The accuracy of the solution is not graded.
- All late assignments are accepted up to one week later at 50% credit.

Grades

Grades	Item	Description
35%	Problem set submission	To be submitted online before the class
35%	Participation	Presenting and explaining the solution of problem set
10%	Project proposal	1 page summary of the project
20%	Project presentation	15-minute presentation of the project
100%	Total	