ARTIFICIAL INTELLIGENCE FOR CLIMATE CHANGE MITIGATION ROADMAP (SECOND EDITION)

CHAPTER 13:

MATERIALS INNOVATION

Colin McCormick

November 2024

Innovation for Cool Earth Forum

CHAPTER 13:

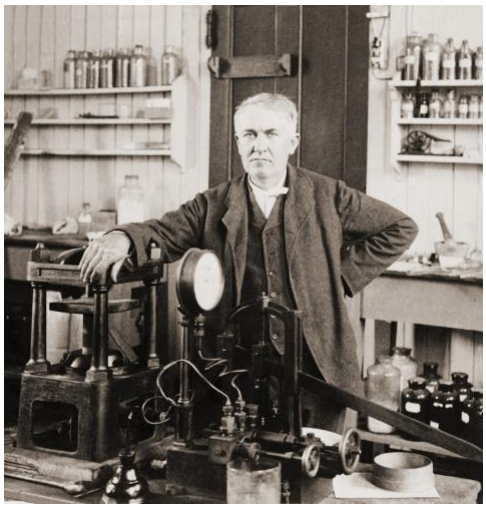
MATERIALS INNOVATION

Colin McCormick

Materials innovation is important for decarbonization, and artificial intelligence (AI) can play a major role in accelerating it. This chapter examines how improved materials can reduce emissions and enable carbon management, as well as specific areas in which AI can help.

Roman concrete enabled extraordinary construction projects, including the Pantheon, the world's oldest building still in active use.

The search for novel materials with useful properties has been central to technology innovation for centuries. Ancient Romans developed novel concrete for bridges, aquifers and other structures, some of which have survived for millennia.[1] In the modern era, Thomas Edison's discovery of carbon filament for electric light bulbs in 1879 enabled these bulbs to last for long enough to be practical, leading to a fundamental transformation of lighting technologies and the eventual phase-out of whale oil and kerosene lamps.[2] Similarly, Charles Goodyear's discovery of a process to vulcanize rubber in the 1830s helped overcome the limitations of natural rubber, which melts in heat and cracks in cold. Goodyear (among others) worked for years to address this challenge, eventually discovering how to cross-link the long molecules in natural rubber to create a much stronger and more durable material.[3]



Thomas Edison's discovery of carbon filament for electric light bulbs in 1879 fundamentally transformed lighting.

These examples illustrate that most materials innovation throughout history has relied on insight, experimentation and serendipity. Edison's search for an appropriate filament depended on general scientific insight and exhaustive material testing: his laboratory tried thousands of carbonized plants before finally identifying one that worked well. Goodyear's discovery of vulcanization was largely due to a stroke of luck. Many other key materials—including carbon steel, ceramics, catalysts and polymers—have followed similar paths. Without a systematic, quantitative framework for determining how a material's properties depend on its chemical and structural nature, there is only one feasible approach: innovators must laboriously find or synthesize many different materials (or many variations of the same basic material with slight modifications) and exhaustively test them. This is costly and time-consuming and creates a barrier to technological progress.

A. Materials innovation in Climate Technologies

The performance of many clean-energy technologies is limited by the properties of key materials, including photovoltaics (PVs), semiconductors, magnets, catalysts, polymers, alloys and composites. Identifying new materials with improved properties could enable these technologies to achieve higher energy efficiency, lower costs, greater performance, longer service lifetime, higher energy densities and many other desirable characteristics. This in turn would allow these technologies to provide identical or improved services with lower net greenhouse gas emissions (GHG).

Materials innovation enabled the development of lithium-ion batteries for electric vehicles (EVs), long-duration grid storage and other low-carbon technologies.

Lithium-ion batteries are a good example of a technology that was greatly improved through discovery of novel materials. Specifically, the cathode, anode and electrolyte materials in modern lithium-ion batteries are all the result of extensive fundamental and applied research. This includes identification of lithium cobalt oxide ($LiCoO_2$), lithium iron phosphate ($LiFePO_4$) and other cathode materials beginning in the 1970s, as well as identification of graphite for anodes and a variety of liquid and solid materials for the electrolyte.[4] Before these materials were identified and successfully integrated into full systems, the performance of batteries was much worse than today (lower energy density and total capacity). The cost of building battery-enabled technologies was correspondingly higher. Advances in these key materials therefore improved performance and thus brought batteries into new applications, such as electric vehicles (EVs) and bulk storage of renewable electricity. Research into advanced battery materials is still ongoing and may open a path to even higher-performing batteries, such as all-solid-state[5] and sodium-ion technologies.[6]

Solar photovoltaic (PV) systems are the product of years of materials innovation and optimization.

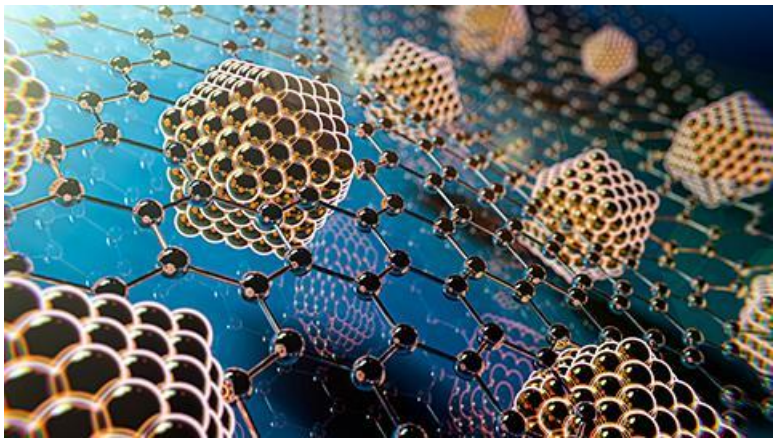
Advanced materials also play important roles in carbon capture and management technologies. Properties such as CO_2-binding energy and kinetics, as well as long-term stability, determine the overall performance of materials used as sorbents and solvents for carbon capture and direct air capture (DAC) applications.[7] Similar properties also determine the performance of catalyst materials in applications such as electrocatalytic reduction of CO_2.[8] Even in the case of CO_2 transport for sequestration or utilization, material properties influence the durability and overall performance of bulk transport systems. [9]

Box 13-1

INNOVATION IN MATERIALS SYNTHESIS

In some cases, a well-known material with superior properties could potentially overcome limitations to a technology's performance, but no practical method is known for producing this material. One such case is the general illumination LED bulb, now in common use. Although LEDs were originally invented in the 1960s, they were based on a material (gallium arsenide, GaAs) that can only emit red light. Researchers knew that gallium nitride (GaN) and zinc selenide (ZnSe) could enable white LEDs that could be used for general applications like building and street lighting. However, it was not until the development of the two-flow MOCVD (metal organic chemical vapor deposition) reactor in the 1990s that GaN crystals could be reliably produced.[10]

This development led directly to commercial, white-colored LED lights with dramatically higher energy efficiency than incandescent and fluorescent bulbs, which are now gradually being replaced. Notably, although LEDs have reduced the energy intensity of lighting significantly, global CO_2 emissions from lighting have not fallen because the demand for more lighting has offset these efficiency gains.[11]



There are many other use cases of advanced materials that are, or would be, valuable in enabling technologies to reduce GHG emissions in energy, industrial, transportation and other applications. These include solar PVs,[12] wind turbine blades,[13] hydrogen storage,[14] fuel-cell electrodes and electrolytes,[15] lightweight alloys and composites for vehicles,[16] low-GWP (global warming potential) refrigerants,[17] thermal-barrier coatings,[18] desiccants for advanced HVAC,[19] high-voltage direct-current (HVDC) power transmission,[20] high-temperature superconductors,[21] and high-strength permanent magnets (used in everything from wind turbines to fusion reactors).[22]

Innovative materials are important for enabling point-source carbon capture systems and CO_2 removal systems, such as this direct air capture (DAC) plant in Iceland (photo credit: Julio Friedmann).

B. Computational Materials Development

Key scientific advances in the 1960s changed the way materials are designed and discovered. New computational methods finally enabled researchers to go beyond simply relying on intuition and incremental experiments; these methods allowed them to directly calculate the properties of new materials just from their chemical makeup and structure ("*ab initio*"). For example, following the discovery of the first high-temperature superconductor (which was largely an Edisonian process guided by intuition), other researchers quickly applied computational modeling to better understand the superconducting effect. This approach led to the discovery of other, better high-temperature superconductors.[23,24] *Ab initio* modeling also led to materials discoveries for batteries, hydrogen storage, thermoelectrics, nuclear fuels and semiconductors.[25]

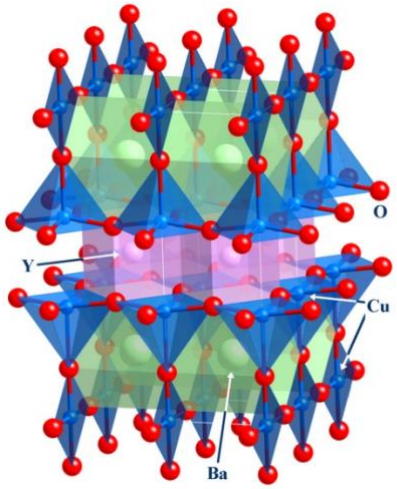
As a result, materials research has increasingly shifted to computation. Advances in computing power, algorithms and data science have accelerated this trend. Governments have funded broadly integrated materials science projects that leverage information-science tools to share advanced algorithms, provide compute resources and disseminate the results of computations and experiments in increasingly massive materials property databases. Some examples include The Materials Project coordinated by U.C. Berkeley,[26] the NOMAD database hosted by Humboldt University of Berlin,[27] and the MateriApps project hosted by the University of Tokyo.[28] These projects

contain hundreds of thousands to millions of entries on material properties and provide methods for users to run numerical calculations of materials properties on high-performance computers. The scale of materials datasets is a consequence of the enormous number of stable materials that could theoretically exist by the laws of chemistry and physics (estimated to be more than the number of atoms on Earth[29]), even though only a tiny fraction of these have actually been synthesized.

Notably, modern computational materials science consumes enormous computing resources. In recent years, roughly one-third of available supercomputing has been dedicated to these materials-related calculations.[30]

C. Applications of AI in Materials Discovery and Design

The complex nature of materials property predictions and the enormous amount of available data have sparked interest in using AI methods in computational materials science for several years. One key area where AI has been applied is directly predicting properties of new materials without performing full *ab initio* calculations. This approach trains AI models on large databases of previously computed and/or tested materials to learn quantitative relationships between atomic structure and relevant properties. This can save enormous compute time and cost. A recent application of this was the use of graph neural networks trained on data from the Materials Project to screen 31 million hypothetically possible crystal structures to identify roughly two thousand of them with promising properties for further investigation.[31] This AI approach can provide major benefits by down-selecting a small number of candidate materials for more intensive, high-accuracy studies. An important recent variation of this approach combined AI algorithms with *ab initio* calculations to generate and then filter potential new inorganic crystals, discovering more than 380,000 new, previously unknown stable materials.[32]



Yttrium barium copper oxide (YBCO) was one of the first high-temperature superconductors to be discovered. Image was created using published crystallographic information and the Crystalmaker® program. Author: Gadolinist

This type of materials prediction and screening relies on large datasets, so ongoing efforts to develop AI-ready massive materials datasets are crucial. The recently released Open DAC 2023 dataset containing millions of high-accuracy calculations of the properties of thousands of sorbent materials

for DAC is a good example of this kind of dataset, enabling multiple teams to train AI models for more extensive and focused rapid materials discovery for DAC.[33]

While *ab initio* calculations will probably remain the most accurate method of predicting materials properties for some time, AI methods have begun to produce impressive results compared to first-principles calculations. For example, an artificial neural network was recently developed to predict key characteristics of the surfaces of binary and ternary oxides, materials that may be useful as PVs and photocatalysts.[34] AI can also be used to accelerate experimental characterization of materials, leading to much more efficient use of limited experimental resources. For example, x-ray diffraction (XRD), which measures the pattern of diffraction of x-rays that hit a sample, is a common technique for examining the crystal structure of materials (such as changes in cathode phases during battery charging). AI models trained on large experimental datasets of diffraction patterns and material crystal structures can directly interpret new XRD data in real time, dramatically speeding up experiments.[35]

An enormous amount of prior materials research is available in scientific journal articles. Researchers typically survey the scientific literature before approaching a new problem, but the large number of relevant articles (often tens of thousands for a single material subtype) makes this process extremely difficult and prone to error and bias. AI in the form of natural language processing (NLP) can be used to extract information from these research articles and structure it systematically, known as "knowledge discovery."[36,37] NLP models trained on non-technical language struggle to handle scientific text, but materials-research-specific language models with better performance have begun to emerge.[38] With the broad introduction of large language models (LLMs) in 2022, progress in materials-science knowledge discovery has begun to accelerate dramatically.[39]

The complexity of advanced materials means that the process used to synthesize (produce) them must be tightly controlled. Small changes in process parameters can result in different, less useful materials, so identifying and optimizing synthesis parameters is crucial. AI-based knowledge-discovery techniques have been successfully applied to the materials research literature to identify precise synthesis steps for key materials from thousands of research papers. For example, researchers used a neural-network-based NLP method to search 22,000 journal articles and extract precise synthesis parameters for optimized titania nanotubes.[40]

Researchers are increasingly working to combine these use cases in integrated "autonomous materials" laboratories. These laboratories combine novel material formulations discovered by AI with physical synthesis guided by specific steps that other AI models summarize from the scientific literature. One recent example allowed the direct synthesis and testing of 41 novel compounds over 17 continuous days of operation.[41] However, designing these autonomous materials laboratories is challenging and requires new thinking about reproducibility and robust handling of various types of errors that can occur in real-world experimental settings.[42] Ultimately, these types of laboratories should aim to achieve a positive feedback loop that integrates AI-guided theoretical materials design, automated chemical synthesis of physical samples, and automated materials characterization.[43]

The use of generative AI is also growing rapidly within materials discovery and design. Generative AI can propose new hypothetical materials that are not currently in any materials database and may be

dramatically different from those that are. This is particularly powerful for the "inverse design" problem of materials, which starts with a desired property and uses an AI method to propose possible materials structures that may have it. As an example, researchers used a generative adversarial network (GAN) to propose 23 entirely novel structures made from three atoms (magnesium, manganese and oxygen) that displayed excellent properties as photoanodes for water splitting.[44] Similarly, researchers recently used a generative AI method to rapidly design and partially validate novel materials for carbon capture, identifying six candidates with very high capacity for further testing.[45]

D. Barriers

Some important progress has already been made in applying AI techniques to computational materials discovery and design. Expanded research budgets, including additional funding for AI-specific applications in materials science, would make even more progress possible.

While high-speed internet connections have partly equalized access to materials datasets and high-performance computing across the globe (with notable exceptions), the same is not true for physical materials-testing facilities. Real breakthroughs will ultimately depend on coupling AI-enabled computational materials discovery with high-throughput synthesis and testing/characterization.

The vast and growing network of materials databases also poses a challenge for progress. Better integration of these datasets, including better harmonization of their metadata, is needed. This would improve the ability of researchers to train models and query materials properties across the full spectrum of existing data, avoiding silos and misinterpretations due to conflicting definitions. Explicitly encouraging inclusion of null results or failed experiments on materials—an uncommon step in most scientific research—could broaden the value of these datasets and provide more balanced training data for AI models. Governments have difficulty acting on these issues unilaterally since the global materials-science community must align on data exchange and metadata protocols. However, international standards bodies and scientific societies can lead the way through cooperative standards-setting efforts, potentially with government funding for support.[46]

At a system level, the full life-cycle emissions implications of advanced materials are dependent on both the key property of interest (e.g., PV efficiency, CO_2-adsorption capacity, etc.) and the emissions caused by synthesizing (producing) the material. Unfortunately, relatively little attention has been paid to synthesis emissions when discovering or optimizing novel materials, even though different synthesis pathways can have significantly different emissions.[47] More use of AI tools is needed in predicting GHG emissions that would be caused by synthesizing novel materials, preferably in parallel with materials discovery and design efforts. This application of AI would allow better understanding of the complete life-cycle emissions that would result from using a novel material in energy and related technologies.

Finally, advances in accelerating materials discovery and design with AI depend on improving the AI knowledge and skills of the materials-science workforce. Key issues in AI, such as understanding the applicability of trained AI models to problems outside the domain of their training data and quantifying the uncertainty of model predictions, are challenging and likely unfamiliar to

conventionally trained materials scientists.[46] AI tools should therefore be incorporated as a central part of materials-science education, and training should also be offered to AI experts who are interested in applying their skills to developing novel materials. These education and training efforts could take place within traditional materials-science curricula or as part of external courses that can ensure the most recent models, numerical algorithms and datasets are presented and continually updated.

E. Risks

Powerful AI-enabled tools and techniques developed for materials innovation could be used to advance materials that enable highly emitting activities. For example, these tools could discover new high-temperature alloys for gas turbines[48] or stronger, more durable alloys for drill bits used in oil and gas drilling.[49] This means that advanced AI models for materials innovation may be "dual use" and lead to the development of high-performance materials that lower the cost of emissions-intensive technologies, undermining momentum toward decarbonization. Policy guardrails are unlikely to be sufficient to address this issue. However, because many emerging decarbonized technologies depend on high-performance materials (as noted above), it may be the case that advanced materials-innovation capabilities are, on balance, more beneficial for low-emitting technologies.

Separately, the pursuit of AI-enabled materials innovation at scale will require resources, and the appropriate allocation of research focus areas may be more challenging than in traditional materials-discovery contexts. In particular, the inherent scaling advantages of AI may make it optimal to concentrate research efforts and data into a smaller number of larger research groups than is currently the case. This concentration could lead to "neglected" areas of materials innovation that fall outside of the increasingly centralized research agendas. Reasonable efforts to maintain a diversity of research teams leveraging AI models for materials innovation that are focused on enabling low-emissions technologies should be sufficient to address this risk.

F. Recommendations

1. *National governments should increase R&D budgets for AI-enabled materials discovery, with a focus on holistic design considerations that include full life-cycle GHG emissions. Support should also be made available for creating new automated and partly autonomous materials-testing laboratories in a variety of locations around the world. By combining AI and robotics, these facilities could unlock broad global access to rapid iterations in materials design and testing, reducing the challenges of participating in advanced materials development for researchers in resource-limited countries.*[50]
2. *Private companies should engage directly with AI-guided materials-discovery efforts by clarifying manufacturability constraints and offering embedded emissions guidelines. This could also include articulating specific materials classes of interest for commercially relevant low-carbon technologies and issuing benchmarks and/or targets for key performance thresholds.*
3. *National governments, academia and private companies should collaborate to develop and release (or expand existing) AI-ready datasets of material properties that can be used by other research teams to train high-performance models. This effort should use standard data formats and be at least loosely coupled to materials-synthesis and -testing facilities to validate results.*
4. *National governments and academia should support increased education in AI techniques as part of materials-science and related degree programs.*
5. *Scientific publishers should ensure that research publications are fully compatible with AI-guided research synthesis methods, including retroactively converting historical publications.*

G. References

1 Seymour 2023. Hot mixing: Mechanistic insights into the durability of ancient Roman concrete. 1-13 (2023). https://www.science.org/doi/10.1126/sciadv.add1602

2 Rebecca Matulka & Daniel Wood. *History of the Light Bulb;* DOE, https://www.energy.gov/articles/history-light-bulb (2013).

3 Cai Guise-Richardson. Redefining Vulcanization: Charles Goodyear, patents, and industrial control, 1834-1865. *Technology and Culture* 51, 357-387 (2010). https://doi.org/10.1353/tech.0.0437.

4 M. V. Reddy *et al.* Brief History of Early Lithium-Battery Development. *Materials (Basel)* 13 (2020). https://doi.org/10.3390/ma13081884.

5 Jürgen Janek & Wolfgang G. Zeier. Challenges in speeding up solid-state battery development. *Nature Energy* 8, 230-240 (2023). https://doi.org/10.1038/s41560-023-01208-9.

6 Ivana Hasa, Nuria Tapia-Ruiz & Montserrat Galceran. Editorial: Sodium-ion batteries: From materials discovery and understanding to cell development. *Frontiers in Energy Research* 10 (2022). https://doi.org/10.3389/fenrg.2022.1076764.

7 Tanay Sahu, Kulbir K. Ghuman & Paul G. O'Brien. in *Progress in Sustainable Development* (eds David Ting & Paul O'Brien) 205-232 (Elsevier, 2023, https://doi.org/10.1016/B978-0-323-99207-7.00003-8).

8 Yuhou Pei, Heng Zhong & Fangming Jin. A brief review of electrocatalytic reduction of CO2—Materials, reaction conditions, and devices. *Energy Science & Engineering* 9, 1012-1032 (2021). https://doi.org/10.1002/ese3.935.

9 Luca Ansaloni, Ben Alcock & Thijs A. Peters. Effects of CO2 on polymeric materials in the CO2 transport chain: A review. *International Journal of Greenhouse Gas Control* 94, 102930 (2020). https://doi.org/10.1016/j.ijggc.2019.102930.

10 Shuji Nakamura. Background story of the invention of efficient blue InGaN light emitting diodes (Nobel Lecture). *Annalen der Physik* 527, 335-349 (2015). https://doi.org/10.1002/andp.201500801.

11 Kevin Lane. *LIGHTING;* https://www.iea.org/energy-system/buildings/lighting (accessed October 2024).

12 Modupeola Dada & Patricia Popoola. Recent advances in solar photovoltaic materials and systems for energy storage applications: a review. *Beni-Suef University Journal of Basic and Applied Sciences* 12, 66 (2023). https://doi.org/10.1186/s43088-023-00405-5.

13 A. V. Pradeep *et al.* A comprehensive review on contemporary materials used for blades of wind turbine. *Materials Today: Proceedings* 19, 556-559 (2019). https://doi.org/10.1016/j.matpr.2019.07.732.

14 Michael Hirscher *et al.* Materials for hydrogen-based energy storage – past, recent progress and future outlook. *Journal of Alloys and Compounds* 827, 153548 (2020). https://doi.org/10.1016/j.jallcom.2019.153548.

15 Ahmed Sajid *et al.* A perspective on development of fuel cell materials: Electrodes and electrolyte. *International Journal of Energy Research* 46, 6953-6988 (2022). https://doi.org/10.1002/er.7635.

16 Wen Zhang & Jun Xu. Advanced lightweight materials for Automobiles: A review. *Materials & Design* 221, 110994 (2022). https://doi.org/10.1016/j.matdes.2022.110994.

17 D. C. Savitha *et al.* Refrigerants for sustainable environment – a literature review. *International Journal of Sustainable Energy* 41, 235-256 (2022). https://doi.org/10.1080/14786451.2021.1928129.

18 S. T. Vagge & Suraj Ghogare. Thermal barrier coatings: Review. *Materials Today: Proceedings* 56, 1201-1216 (2022). https://doi.org/10.1016/j.matpr.2021.11.170.

19 R. P. Singh, V. K. Mishra & R. K. Das. Desiccant materials for air conditioning applications - A review. *IOP Conference Series: Materials Science and Engineering* 404, 012005 (2018). https://dx.doi.org/10.1088/1757-899X/404/1/012005.

20 Christoph Felix Niedik *et al.* Improvement of high voltage direct current material properties upon tailoring the morphology of crosslinked polyethylenes. *Polymer Crystallization* 4, e10208 (2021). https://doi.org/10.1002/pcr2.10208.

21 Alexander Molodyk & David C. Larbalestier. The prospects of high-temperature superconductors. *Science* 380, 1220-1222 (2023). https://doi.org/10.1126/science.abq4137.

22 J. M. D. Coey. Perspective and Prospects for Rare Earth Permanent Magnets. *Engineering* 6, 119-131 (2020). https://doi.org/10.1016/j.eng.2018.11.034.

23 J. Georg Bednorz & K. Alex Müller. Perovskite-Type Oxides—the New Approach to High-Tc Superconductivity. Nobel Lecture. *Angewandte Chemie International Edition in English* 27, 735-748 (1988). https://doi.org/10.1002/anie.198807351.

24 Warren E. Pickett. Electronic structure of the high-temperature oxide superconductors. *Reviews of Modern Physics* 61, 433-512 (1989). https://doi.org/10.1103/RevModPhys.61.433.

25 R. Ramprasad *et al.* Recent advances in first principles computations in materials research. *Journal of Materials Science* 47, 7313-7316 (2012). https://doi.org/10.1007/s10853-012-6736-0.

26 The Materials Project. *The Materials Project: A materials genome approach to accelerating materials innovation;* https://next-gen.materialsproject.org/ (Acessed August 2024).

27 NOMAD. *Materials science data managed and shared;* Humbolt University of Berlin, https://nomad-lab.eu/nomad-lab/ (2023).

28 University of Tokyo. *MateriApps;* https://ma.issp.u-tokyo.ac.jp/en (2023).

29 Peter Kirkpatrick & Clare Ellis. Chemical space. *Nature* 432, 823-823 (2004). https://doi.org/10.1038/432823a.

30 Stefan Heinen *et al.* Machine learning the computational cost of quantum chemistry. *Machine Learning: Science and Technology* 1, 025002 (2020). https://doi.org/10.1088/2632-2153/ab6ac4.

31 Chi Chen & Shyue Ping Ong. A universal graph deep learning interatomic potential for the periodic table. *Nature Computational Science* 2, 718-728 (2022). https://doi.org/10.1038/s43588-022-00349-3.

32 Amil Merchant *et al.* Scaling deep learning for materials discovery. *Nature* 624, 80-85 (2023). https://doi.org/10.1038/s41586-023-06735-9.

33 Anuroop Sriram *et al.* The Open DAC 2023 Dataset and Challenges for Sorbent Discovery in Direct Air Capture. *ACS Central Science* 10, 923-941 (2024). https://doi.org/10.1021/acscentsci.3c01629.

34 Shin Kiyohara, Yoyo Hinuma & Fumiyasu Oba. Band Alignment of Oxides by Learnable Structural-Descriptor-Aided Neural Network and Transfer Learning. *Journal of the American Chemical Society* 146, 9697-9708 (2024). https://doi.org/10.1021/jacs.3c13574.

35 Nathan J. Szymanski *et al.* Adaptively driven X-ray diffraction guided by machine learning for autonomous phase identification. *npj Computational Materials* 9, 31 (2023). https://doi.org/10.1038/s41524-023-00984-y.

36 Olga Kononova *et al.* Opportunities and challenges of text mining in materials research. *iScience* 24, 102155 (2021). https://doi.org/10.1016/j.isci.2021.102155.

37 Edward O. Pyzer-Knapp *et al.* Accelerating materials discovery using artificial intelligence, high performance computing and robotics. *npj Computational Materials* 8, 84 (2022). https://doi.org/10.1038/s41524-022-00765-z.

38 Tanishq Gupta *et al.* MatSciBERT: A materials domain language model for text mining and information extraction. *npj Computational Materials* 8, 102 (2022). https://doi.org/10.1038/s41524-022-00784-w.

39 Yiwen Hu & Markus J. Buehler. Deep language models for interpretative and predictive materials science. *APL Machine Learning* 1 (2023). https://doi.org/10.1063/5.0134317.

40 Edward Kim *et al.* Materials Synthesis Insights from Scientific Literature via Text Extraction and Machine Learning. *Chemistry of Materials* 29, 9436-9444 (2017). https://doi.org/10.1021/acs.chemmater.7b03500.

41 Nathan J. Szymanski *et al.* An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* 624, 86-91 (2023). https://doi.org/10.1038/s41586-023-06734-w.

42 Zhichu Ren *et al.* Autonomous experiments using active learning and AI. *Nature Reviews Materials* 8, 563-564 (2023). https://doi.org/10.1038/s41578-023-00588-4.

43 Santiago Miret *et al.* Perspective on AI for accelerated materials design at the AI4Mat-2023 workshop at NeurIPS 2023. *Digital Discovery* 3, 1081-1085 (2024). http://dx.doi.org/10.1039/D4DD90010C.

44 Sungwon Kim *et al.* Generative Adversarial Networks for Crystal Structure Prediction. *ACS Central Science* 6, 1412-1420 (2020). https://doi.org/10.1021/acscentsci.0c00426.

45 Hyun Park *et al.* A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture. *Communications Chemistry* 7, 21 (2024). https://doi.org/10.1038/s42004-023-01090-2.

46 Dane Morgan & Ryan Jacobs. Opportunities and Challenges for Machine Learning in Materials Science. *Annual Review of Materials Research* 50, 71-103 (2020). https://doi.org/10.1146/annurev-matsci-070218-010015.

47 Carlos A. Grande *et al.* Life-cycle assessment as a tool for eco-design of metal-organic frameworks (MOFs). *Sustainable Materials and Technologies* 14, 11-18 (2017). https://doi.org/10.1016/j.susmat.2017.10.002.

48 D. Sauceda *et al.* High throughput exploration of the oxidation landscape in high entropy alloys. *Materials Horizons* 9, 2644-2663 (2022). http://dx.doi.org/10.1039/D2MH00729K.

49 Ruizhi Zhong, Cyrus Salehi & Ray Johnson. Machine learning for drilling applications: A review. *Journal of Natural Gas Science and Engineering* 108, 104807 (2022). https://doi.org/10.1016/j.jngse.2022.104807.

50 Nature Synthesis Editorial. Automate and digitize. *Nature Synthesis* 2, 459-459 (2023). https://doi.org/10.1038/s44160-023-00354-y.