

Materials are Mission Critical to the Sustainability Transition: Accelerating Discovery of Materials for Sustainability

Bichlien H Nguyen
Microsoft Research

Artificial intelligence (AI) is rapidly transforming the field of materials science, offering a new paradigm to accelerate the discovery and design of sustainable materials. This article explores how AI-driven innovations are enabling breakthroughs across the material spectrum, from recyclable polymers, coolants, to low-carbon cement and crystalline materials for energy applications – advancing goals across material circularity, clean energy transition, and climate resilience. Additionally, it examines current key bottlenecks in AI for materials design, including computational limitations and data gaps. Finally, the article highlights emerging opportunities to close the loop between theory and practice through agentic AI systems and automation, emphasizing the importance of sustained investment and thoughtful deployment to catalyze a more sustainable future.

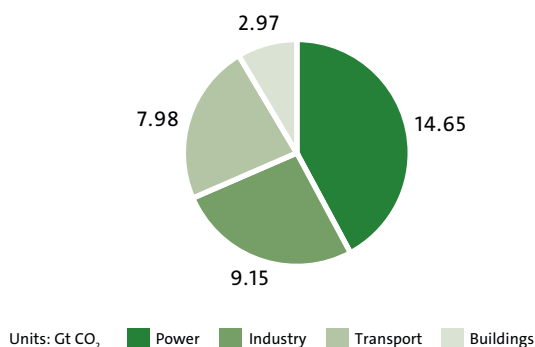
Introduction

Human history is decorated with periods of rapid innovation which manifest in large productivity and efficiency gains across all economic sectors. Since the 1800s, advancements in chemistry, biology, and materials science and engineering have been seamlessly integrated into modern conveniences. Take the simple task of grocery shopping as an example. The groceries we buy depend on a global food production ecosystem that relies heavily on ammonia-based fertilizers produced through the Haber-Bosch process, which is a chemical process that converts nitrogen and hydrogen gas into ammonia using a catalyst.¹ Without the invention of food-grade plastics, packaging and shipping these groceries without spoilage would be nearly impossible at an affordable price. The modern grocery store, itself, is an engineered union of structural materials such as steel and concrete. Behind the scenes, complex supply chains are navigated to distribute fruits and vegetables efficiently across the world to the local supermarket at peak ripeness; all of which would be impossible without computers and countless underlying science and engineering innovations to orchestrate their distribution and transport.

With modern conveniences come modern challenges, however, as there is no such thing as a free lunch. One of the single most energy-intensive chemical reactions, the Haber-Bosch process is estimated to consume a staggering 1% of global energy demand per year to support modern agriculture.³ Plastic production is estimated to produce over 5% of GHG emissions⁴ and current plastic waste is projected to be over 350 Mt, of which less than 10% is recycled.⁵ The production of steel and cement, a critical component in concrete, is estimated to contribute to ~14% of total GHG emissions.⁶ Additionally, there is growing concern about the human and environmental impacts of electronic waste⁷ as well as the high energy intensity of semiconductor production.⁸ Materials and their production, while foundational to global development, are major contributors to climate change with adverse environmental impacts.

The world urgently needs to design novel materials and manufacturing processes that can reduce GHG emissions and improve environmental sustainability goals. Innovations in materials science can reduce environmental impacts in two key ways: first, by developing more sustainable alternatives to existing materials – such as green steel or cement – and second, by developing materials with new capabilities, like advanced batteries for long-duration energy storage or CO₂ capture sorbents for direct air capture.⁹ With artificial intelligence (AI) disrupting whole fields of research from computer science to computational biology,¹⁰ AI presents a transformative opportunity to accelerate materials discovery and optimization to decarbonize the built environment. While AI comes with significant resource and energy costs, it also has real potential for addressing the very sustainability challenges discussed above.¹¹ Here, we discuss the most promising roles AI plays in materials science from materials discovery to educating future sustainability champions whilst addressing current pitfalls and shortcomings of AI in this space.

Figure 1: Global CO₂ emissions by sector, 2022



Source: Adapted from IEA (2023).²



Searching, Designing, and Testing New Materials with AI

Material scientists have long desired to design and synthesize novel materials with predicted properties tailored to specific applications. Referred to as inverse materials design, the core concept utilizes computational methods to enable predictions of a theoretical material and its properties prior to performing physical experiments, which promises to reduce the time and cost required for extensive synthesis and characterization to achieve the desired material. Traditionally, inverse materials design relied on property predictors trained on small experimental datasets. With the widespread adoption of physics-based computational methods, such as density functional theory (DFT) or molecular dynamics (MD), it became possible to predict properties from first principles calculations. These physics-based calculations can be slow and expensive to run for every possible combination of atoms and hence, machine learned (ML) surrogate models trained with synthetic datasets covering the entire periodic table are being developed. As an example, this approach coupled with cloud computing has enabled rapid screening of millions of potential battery materials on Azure Quantum Elements and has led to discovery of a new solid-state lithium-ion electrolyte.¹²

AI-driven inverse design introduces a new paradigm shift for materials design by replacing the traditional screening workflows aimed at specific materials with advanced ML algorithms capable of traversing across complex chemical space from the atomic- to micro- scale. This new paradigm for materials science could enable exploration of all possible materials – an impossible feat with conventional methods – and discover materials critical to reaching 2050 sustainability goals. Below are three examples of how AI is already making tangible impacts in material science.

Microsoft Research in collaboration with the University of Washington demonstrated how AI can be used to guide development of a new bio-based concrete formula that replaces cement with microalgae, leading to a potential 20% reduction in embodied carbon over conventional concrete.

Case Study: Discovering Low-Carbon Concrete

Concrete, a mixture of cement and aggregates, is a ubiquitous building material that has been optimized for its structural properties over centuries. Reducing or replacing the carbon intensive cement in concrete while maintaining its structural properties could significantly reduce global GHG emissions. AI can help accelerate the discovery of new concrete mixtures. Using a conditional variational autoencoder (CVAE) conditioned on compressive strength and environmental impacts, Meta optimized a new concrete formulation that could potentially reduce embodied carbon of concrete by up to 40% while maintaining its structural properties.¹³ Recently, Microsoft Research in collaboration with the University of Washington demonstrated how AI can be used to guide development of a new bio-based concrete formula that replaces cement with microalgae, leading to a potential 20% reduction in embodied carbon over conventional concrete.¹⁴

Case Study: Designing New Recyclable Plastics

Plastics are a family of carbon-based, amorphous materials primarily derived from petrochemicals.^{15, 16, 17} They are comprised of repeating monomer units that are linked together to form polymer chains which can be generally processed as linear or cross-linked plastics depending on the specific polymer chemistry. Cross-linked plastics have unique properties that favor their use in advanced composites such as printed circuit boards and structural components like wind turbines. Unlike their linear counterparts, cross-linked plastics are historically non-recyclable. Recently, a new class of polymers called vitrimers has been proposed that maintain the technical performance of cross-linked polymers while retaining the ability to recycle. Microsoft Research and the University of Washington demonstrated that vitrimers could be used to make recyclable composites in electronics,¹⁸ enabling recovery and reuse of integrated circuits and copper from printed circuit boards. The team further demonstrated that these polymers could be optimized to improve their thermal stability without compromising other properties such as recyclability with generative AI.¹⁹

Case Study: Generating New Crystalline Materials

Inorganic crystalline materials are found in a wide variety of applications such as semiconductors, batteries, photovoltaics, and turbines. Some notable examples are silicon, indium tin oxide, cadmium telluride, and neodymium magnets. The structure or arrangement of atoms in a crystal lattice structure along with the elements in the composition determines many properties of the crystal. Predicting the exact composition and structure of inorganic crystals with desired properties could enable development of cheaper, more efficient energy materials. For example, Google Deepmind's GNoME

model employed graph neural networks (GNNs) to screen a large library of crystal structures in an active learning loop to predict over 300,000 computationally stable materials.²⁰ In another approach, Microsoft Research AI for Science trained a generative model for inorganic crystals, MatterGen,²¹ which can be fine-tuned to predict stable, novel materials with targeted properties across the periodic table. In combination with MatterSim, a machine learned surrogate model for prediction of energy and forces of atoms, the team predicted new crystalline materials with high magnetic density containing no rare earth elements as a first step toward a new family of magnets.

Challenges in AI for Sustainable Materials Design

Mind the Computational Gap

Computational predictions – whether of organic molecules, polymers, or inorganic crystals – are only the first step in materials discovery. A structure must be synthesized to become a realized material, and its properties must be experimentally verified to be considered functional. Successfully creating a new material depends on two main factors: its stability – determined by thermodynamics – and how readily it forms – determined by kinetics. Yet, because kinetics modeling is computationally challenging and costly, AI property predictors are typically trained to predict only thermodynamic properties because these synthetic datasets can be more easily generated from computational workflows such as DFT or MD. This limits their ability to predict experimentally viable outcomes and hinders modeling of rate-dependent processes such as catalysis.

Furthermore, the accuracy of AI models used to predict material properties depend heavily on the accuracy of the physics-based computational workflows used to generate their training data. For instance, DFT methods estimate electron-electron interactions in a material while MD simulates the movement and interaction of atoms. Both methods involve approximations which can introduce and compound errors in AI models. However, recent advances in deep learning algorithms offer promising solutions. By learning a more accurate mathematical representation for electron interactions in DFT^{22, 23} and improving the accuracy of atomic interaction models in MD,^{24, 25} errors in synthetic datasets can be reduced and enable more accurate AI property predictors.

The Need for Data and Diversity

Efficiencies in high performance computing have reduced the cost and increased the speed of generating large synthetic datasets for training AI models in material science. This has spurred creation of initiatives such as the Materials Project²⁶ and Meta’s Open Catalyst Project²⁷ where computational workflows, ML models,

and datasets are openly available to the public under findable, accessible, interoperable, and reusable (FAIR) principles. In the age of large foundation models, data has been recognized as independently valuable and open-sourcing expensive-to-generate datasets is often disincentivized. Open-sourcing workflows and datasets, however, remains critical for scientific reproducibility and interoperability,²⁸ and the community needs to ensure a good balance is struck to ensure continued innovation in this field.

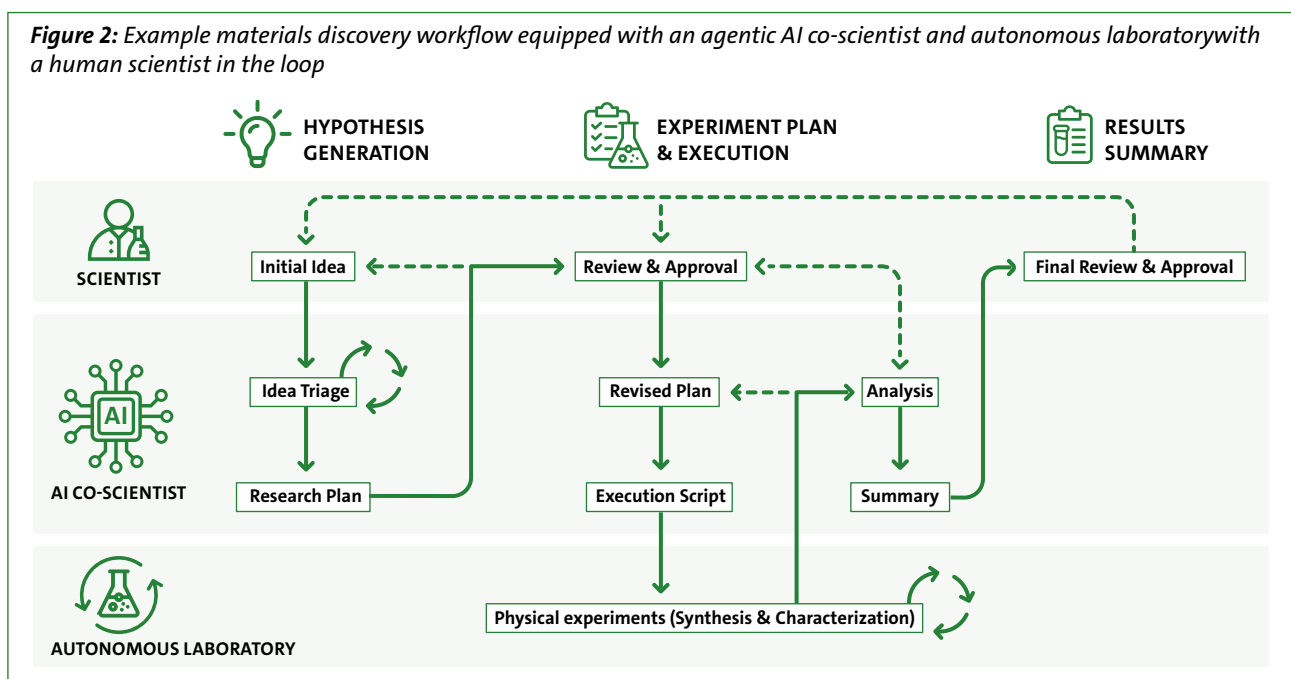
In addition to sparse workflows and data availability, most large AI training datasets in materials science focus on atomic properties based on structure and composition of the material. While certain properties such as electronic bandgaps, ionization potentials, and bulk modulus can be calculated using quantum chemistry workflows, many relevant real-world properties are determined at different length scales. For structural materials, the microstructure of the material determines important properties such as ductility, strength, and corrosion resistance. Computational workflows and synthetic and experimental data in these length regimes are sparse but needed to predict real materials and processes.²⁹

Materials do not Exist in a Vacuum

Sustainability is an inherently interdisciplinary field, spanning from basic science to policy, and requires thinking about interacting systems at scale. No single algorithm or material will be the silver bullet that unlocks the gateway to a more sustainable future. Materials discovery, selection, and engineering must be evaluated in relation to the larger industrial ecosystems in which they reside to accelerate adoption of more sustainable technologies.³⁰ Using AI to accelerate materials research at all length scales is key, and emphasis on developing AI systems to accelerate the process and engineering of materials and to evaluate new materials at the device scale should be encouraged to bridge technology readiness gaps. AI could be a key driver in developing an informed workforce capable of amalgamating opportunities, tradeoffs, and externalities of new material innovations and promote their integration into technologies, whilst navigating complex logistics, economic and regulatory landscapes.^{31, 32}

Looking Forward to Closing the Loop with Automation

Figure 2: Example materials discovery workflow equipped with an agentic AI co-scientist and autonomous laboratory with a human scientist in the loop



Research agents

Materials discovery is an arduous, complex process guided by the scientific method – an iterative feedback loop of observations, questions, hypotheses, experiments, analysis, and conclusions. It is becoming possible to develop agentic AI systems that can assist researchers at each stage of the scientific method. A typical first-generation co-scientist has a natural language interface with which users can prompt and interact with the system, access to domain-specific tools, modules, and agents, can execute asynchronous, continuous, and configurable downstream tasks, and has contextual memory from which it can be used to improve subsequent tasks.³³ Early examples of co-scientist experiments have been reported by Google³⁴ and Microsoft Discovery.³⁵ Notably, Microsoft Discovery demonstrated the use of their agentic platform to discover alternative coolants to polyfluoroalkyl substances (PFAS) for next generation datacenter cooling applications. Usage of PFAS is under threat of global bans and development of new coolants could help datacenter operations reduce GHG emissions by 20%.³⁶ As AI models become increasingly more capable, AI co-scientists have the potential to significantly reduce the timeline to new materials discovery, especially if coupled with rapid experimental capabilities.

As AI models become increasingly more capable, AI co-scientists have the potential to significantly reduce the timeline to new materials discovery, especially if coupled with rapid experimental capabilities.

Autonomous Laboratories

Experimental validation is critical to determining the functionality of predicted materials, and integrating AI-enabled materials design with autonomous experimental synthesis represents a major leap forward to bridging computational and experimental approaches for materials discovery.³⁷ The main advantage of automation is the ability to acquire high-throughput experimental data which then can act as ground truth for computational predictions.³⁸ An AI-enabled autonomous laboratory, however, can go beyond acquiring experimental data. Notable examples in this burgeoning space are the University of Berkeley's A-Lab³⁹ for inorganic materials, University of Liverpool's autonomous platform for chemistry,⁴⁰ and Argonne National Laboratory's PolyBot⁴¹ for development of polymeric thin films. By incorporating a large corpus of literature data and ML models coupled with robotics, AI-enabled autonomous platforms have been shown to predict materials, create synthesis plans, execute the synthesis, perform characterization, and reason through the entire experimental run. As autonomous capabilities advance, the rate of materials discovery is expected to increase.

Conclusion

Materials are the cornerstone of our built environment, and their design, use, production, and disposal are deeply entrenched within our global environmental footprint. The convergence of AI and materials science offers a unique opportunity to accelerate the deployment of sustainable material innovations, where functional materials can be designed and optimized for technical and environmental benefits. Despite challenges such as limited data diversity and computational gaps, AI has shown early promise in rapidly narrowing down the search space of potential candidates from biodegradable polymers to low-carbon concrete and crystalline materials for energy storage, reducing the time for new material discovery. Yet, discovery is just the first step. Real-world impact in sustainability requires rigorous experimental validation, thoughtful integration into global ecosystems, and most importantly – time. Harnessing the full potential of AI for sustainability will not happen overnight. It takes time to synthesize, characterize, and deploy new materials. It takes time to build trust, infrastructure, and policy frameworks that support adoption, and it takes time to cultivate the human expertise needed to guide AI responsibly and effectively. Only through continuous investment in AI and a commitment to closing the loop between theory and practice can we catalyze a more sustainable future.



Crystalline materials

About the author

Bichlien Nguyen is principal researcher at Microsoft in Redmond, WA and an affiliate assistant professor at the Department of Computer Science and Engineering at the University of Washington. Working at the intersection of chemistry, biology, computer science, and electrical engineering, her research interests are in developing AI technology to accelerate the development of sustainable infrastructure, from materials design to systems modeling.

- 1 Chemical & Engineering News. (2023). *The industrialization of the Haber–Bosch process*. <https://cen.acs.org/food/agriculture/The-industrialization-Haber-Bosch-process/101/i26>
- 2 International Energy Agency. (2023). Global CO₂ emissions by sector, 2019–2022 [Data set]. <https://www.iea.org/data-and-statistics/charts/global-co2-emissions-by-sector-2019-2022>
- 3 Chemical & Engineering News. (2019). *Industrial ammonia production emits more CO₂ than any other chemical-making reaction*. <https://cen.acs.org/environment/green-chemistry/Industrial-ammonia-production-emits-CO2/97/i24>
- 4 Karali, N., Khanna, N., & Shah, N. (2024). *Climate impact of primary plastic production*. Lawrence Berkeley National Laboratory. <https://escholarship.org/uc/item/12s624vf>
- 5 Geyer, R., Jambeck, J. R., & Law, K. L. (2017). Production, use, and fate of all plastics ever made. *Science Advances*, 3(7), e1700782. <https://doi.org/10.1126/sciadv.1700782>
- 6 International Energy Agency. (2025a). *Demand and supply measures for the steel and cement transition*. <https://www.iea.org/reports/demand-and-supply-measures-for-the-steel-and-cement-transition>
- 7 World Health Organization. (2021). *Children and digital dumpsites: E-waste exposure and child health*. <https://www.who.int/publications/i/item/9789240024557>
- 8 McKinsey & Company. (2022). *Keeping the semiconductor industry on the path to net zero*. <https://www.mckinsey.com/industries/semiconductors/our-insights/keeping-the-semiconductor-industry-on-the-path-to-net-zero>
- 9 Park, H., Yan, X., Zhu, R., Huerta, E. A., Chaudhuri, S., Cooper, D., Foster, I., & Tajkhorshid, E. (2024). A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture. *Communications Chemistry*, 7(1). <https://doi.org/10.1038/s42004-023-01090-2>
- 10 Abramson, J., Adler, J., Dunger, J., Evans, R., Green, T., Pritzel, A., ... Jumper, J. M. (2024). Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature*, 630(8016), 493–500. <https://doi.org/10.1038/s41586-024-07487-w>
- 11 International Energy Agency. (2025b). *Energy and AI*. <https://www.iea.org/reports/energy-and-ai>
- 12 Chen, C., Nguyen, D. T., Lee, S. J., Baker, N. A., Karakoti, A. S., Lauw, L., ... Troyer, M. (2024). Accelerating computational materials discovery with machine learning and cloud high-performance computing. *Journal of the American Chemical Society*, 146(29), 20009–20018. <https://doi.org/10.1021/jacs.4c03849>
- 13 Ge, X., Goodwin, R. T., Yu, H., Romero, P., Abdelrahman, O., Sudhakar, A., ... Varshney, L. R. (2022). Accelerated design and deployment of low-carbon concrete for data centers. *Proceedings of the ACM SIGCAS/SIGCHI Conference on Computing and Sustainable Societies (COMPASS)*, 340–352. <https://doi.org/10.1145/3530190.3534817>
- 14 Lin, M.-Y., Severson, K., Grandgeorge, P., & Roumeli, E. (2025). Closed-loop optimization using machine learning for the accelerated design of sustainable cements incorporating algal biomatter. *Matter*. <https://doi.org/10.1016/j.matt.2025.102267>
- 15 European Environment Agency. (2020). *Biodegradable and compostable plastics — Challenges and opportunities*. <https://www.eea.europa.eu/en/analysis/publications/biodegradable-and-compostable-plastics>
- 16 Monclús, L., Arp, H. P. H., Groh, K. J., Faltynkova, A., Løseth, M. E., Muncke, J., ... Wagner, M. (2025). Mapping the chemical complexity of plastics. *Nature*, 643(8071), 349–355. <https://doi.org/10.1038/s41586-025-09184-8>
- 17 Rosenboom, J.-G., Langer, R., & Traverso, G. (2022). Bioplastics for a circular economy. *Nature Reviews Materials*, 7(2), 117–137. <https://doi.org/10.1038/s41578-021-00407-8>
- 18 Zhang, Z., Biswal, A. K., Nandi, A., Frost, K., Smith, J. A., Nguyen, B. H., ... Iyer, V. (2024). Recyclable vitrimer-based printed circuit boards for sustainable electronics. *Nature Sustainability*, 7(5), 616–627. <https://doi.org/10.1038/s41893-024-01333-7>
- 19 Zheng, Y., Thakolkaran, P., Biswal, A. K., Smith, J. A., Lu, Z., ... Vashisth, A. (2025). AI-guided inverse design and discovery of recyclable vitrimeric polymers. *Advanced Science*, 12(6). <https://doi.org/10.1002/advs.202411385>
- 20 Merchant, A., Batzner, S., Schoenholz, S. S., Aykol, M., Cheon, G., & Cubuk, E. D. (2023). Scaling deep learning for materials discovery. *Nature*, 624(7990), 80–85. <https://doi.org/10.1038/s41586-023-06735-9>
- 21 Zeni, C., Pinsler, R., Zügner, D., Fowler, A., Horton, M., ... Xie, T. (2025). A generative model for inorganic materials design. *Nature*, 639(8055), 624–632. <https://doi.org/10.1038/s41586-025-08628-5>
- 22 Kirkpatrick, J., McMorrow, B., Turban, D. H. P., ... Cohen, A. J. (2021). Pushing the frontiers of density functionals by solving the fractional electron problem. *Science*, 374(6573), 1385–1389. <https://doi.org/10.1126/science.abj6511>
- 23 Luise, G., Huang, C.-W., Vogels, T., ... Gori-Giorgi, P. (2025). *Accurate and scalable exchange-correlation with deep learning* (arXiv preprint). <https://doi.org/10.48550/arXiv.2506.14665>
- 24 Chmiela, S., Sauceda, H. E., Müller, K.-R., & Tkatchenko, A. (2018). Towards exact molecular dynamics simulations with machine-learned force fields. *Nature Communications*, 9(1). <https://doi.org/10.1038/s41467-018-06169-2>
- 25 Yang, H., Hu, C., Zhou, Y., ... Lu, Z. (2024). *MatterSim: A deep learning atomistic model across elements, temperatures and pressures* (arXiv preprint). <https://doi.org/10.48550/arXiv.2405.04967>
- 26 The Materials Project. (n.d.). *The Materials Project*. <https://next-gen.materialsproject.org/>
- 27 Open Catalyst Project. (n.d.). *Open Catalyst Project*. <https://opencatalystproject.org/>
- 28 MIT Technology Review. (2024). *The race to find new materials with AI needs more data*. <https://www.technologyreview.com/2024/10/18/1105880/the-race-to-find-new-materials-with-ai-needs-more-data-meta-is-giving-massive-amounts-away-for-free/>
- 29 Kovachki, N., Liu, B., Sun, X., Zhou, H., Bhattacharya, K., Ortiz, M., & Stuart, A. (2022). Multiscale modeling of materials. *Mechanics of Materials*, 165, 104156. <https://doi.org/10.1016/j.mechmat.2021.104156>
- 30 Hultman, L., Mazur, S., Ankaracrona, C., ... Berggren, M. (2024). Advanced materials provide solutions towards a sustainable world. *Nature Materials*, 23(2), 160–161. <https://doi.org/10.1038/s41563-023-01778-9>

- 31 Li, B., Mellou, K., Zhang, B., Pathuri, J., & Menache, I. (2023). *Large language models for supply chain optimization* (arXiv preprint). <https://doi.org/10.48550/arXiv.2307.03875>
- 32 Zhong, S., Aseniero, B. A., Groom, A. I., ... Benjamin, D. (2025). Towards interactive AI-assisted material selection for sustainable building design. *Companion Proceedings of the ACM Designing Interactive Systems Conference*, 567–573. <https://doi.org/10.1145/3715668.3736354>
- 33 Boiko, D. A., MacKnight, R., Kline, B., & Gomes, G. (2023). Autonomous chemical research with large language models. *Nature*, 624(7992), 570–578. <https://doi.org/10.1038/s41586-023-06792-0>
- 34 Gottweis, J., Weng, W.-H., Daryin, A., ... Natarajan, V. (2025). *Towards an AI co-scientist* (arXiv preprint). <https://doi.org/10.48550/arXiv.2502.18864>
- 35 Microsoft Discovery. (2025). *Transforming R&D with agentic AI: Introducing Microsoft Discovery*. <https://azure.microsoft.com/en-us/blog/transforming-rd-with-agentic-ai-introducing-microsoft-discovery/>
- 36 Alissa, H., Nick, T., Raniwala, A., ... Frieze, M. (2025). Using life cycle assessment to drive innovation for sustainable cool clouds. *Nature*, 641(8062), 331–338. <https://doi.org/10.1038/s41586-025-08832-3>
- 37 Pyzer-Knapp, E. O., Pitera, J. W., Staar, P. W. J., ... Curioni, A. (2022). Accelerating materials discovery using artificial intelligence, high performance computing and robotics. *npj Computational Materials*, 8(1). <https://doi.org/10.1038/s41524-022-00765-z>
- 38 Delgado-Licona, F., Alsaari, A., Dickerson, H., ... Abolhasani, M. (2025). Flow-driven data intensification to accelerate autonomous inorganic materials discovery. *Nature Chemical Engineering*. <https://doi.org/10.1038/s44286-025-00249-z>
- 39 Szymanski, N. J., Rendy, B., Fei, Y., ... Ceder, G. (2023). An autonomous laboratory for the accelerated synthesis of novel materials. *Nature*, 624(7990), 86–91. <https://doi.org/10.1038/s41586-023-06734-w>
- 40 Dai, T., Vijayakrishnan, S., Szczypiński, F. T., ... Cooper, A. I. (2024). Autonomous mobile robots for exploratory synthetic chemistry. *Nature*, 635(8040), 890–897. <https://doi.org/10.1038/s41586-024-08173-7>
- 41 Wang, C., Kim, Y.-J., Vriza, A., ... Xu, J. (2025). Autonomous platform for solution processing of electronic polymers. *Nature Communications*, 16(1). <https://doi.org/10.1038/s41467-024-55655-3>