AI MEETS MATERIALS

A Renaissance in Materials Discovery

TEMASEK

AI is Unlocking the Door to Endless Possibilities in Materials Discovery

From generating novel material candidates to exploring vast chemical spaces, AI is ushering in a transformative leap in material science.

Through extraordinary speed and precise calculations:

Accelerated Discovery

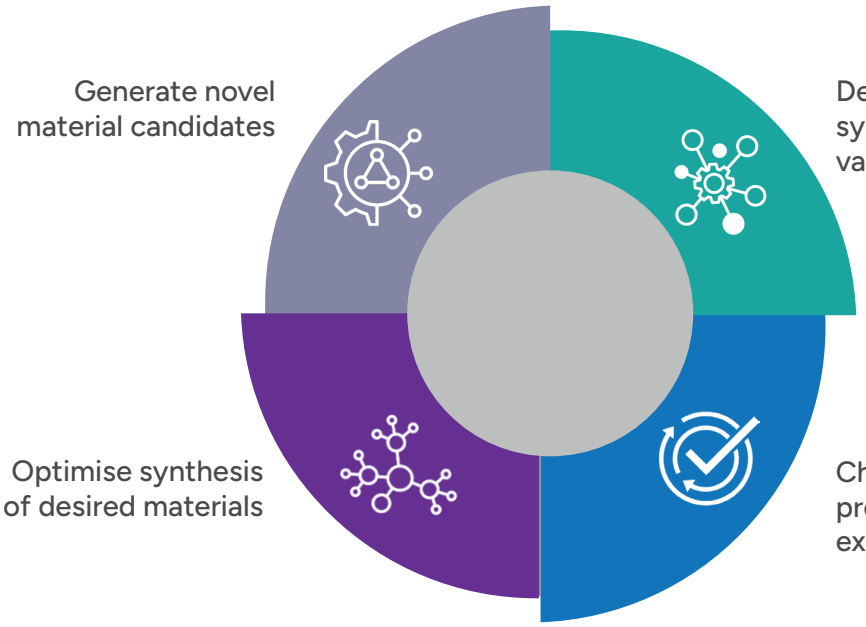
More accurate predictions:

Reduced Cost and Waste

Starting with the desired material properties:

Targeted Discovery and Design

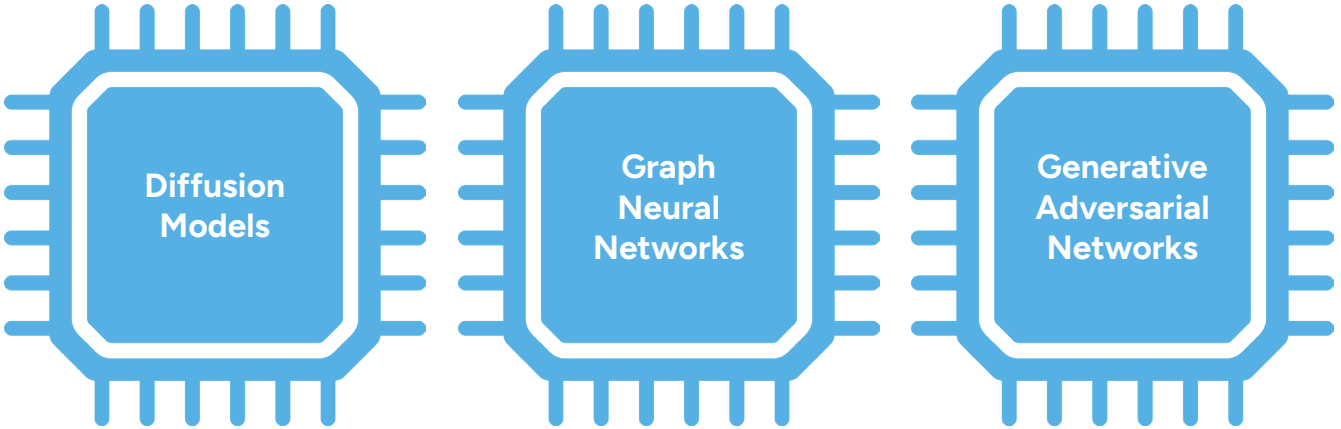
AI can...



...all in a matter of days

AI Methods

Among AI methods, these offer promising potential noting their neural network backbone.



Challenges

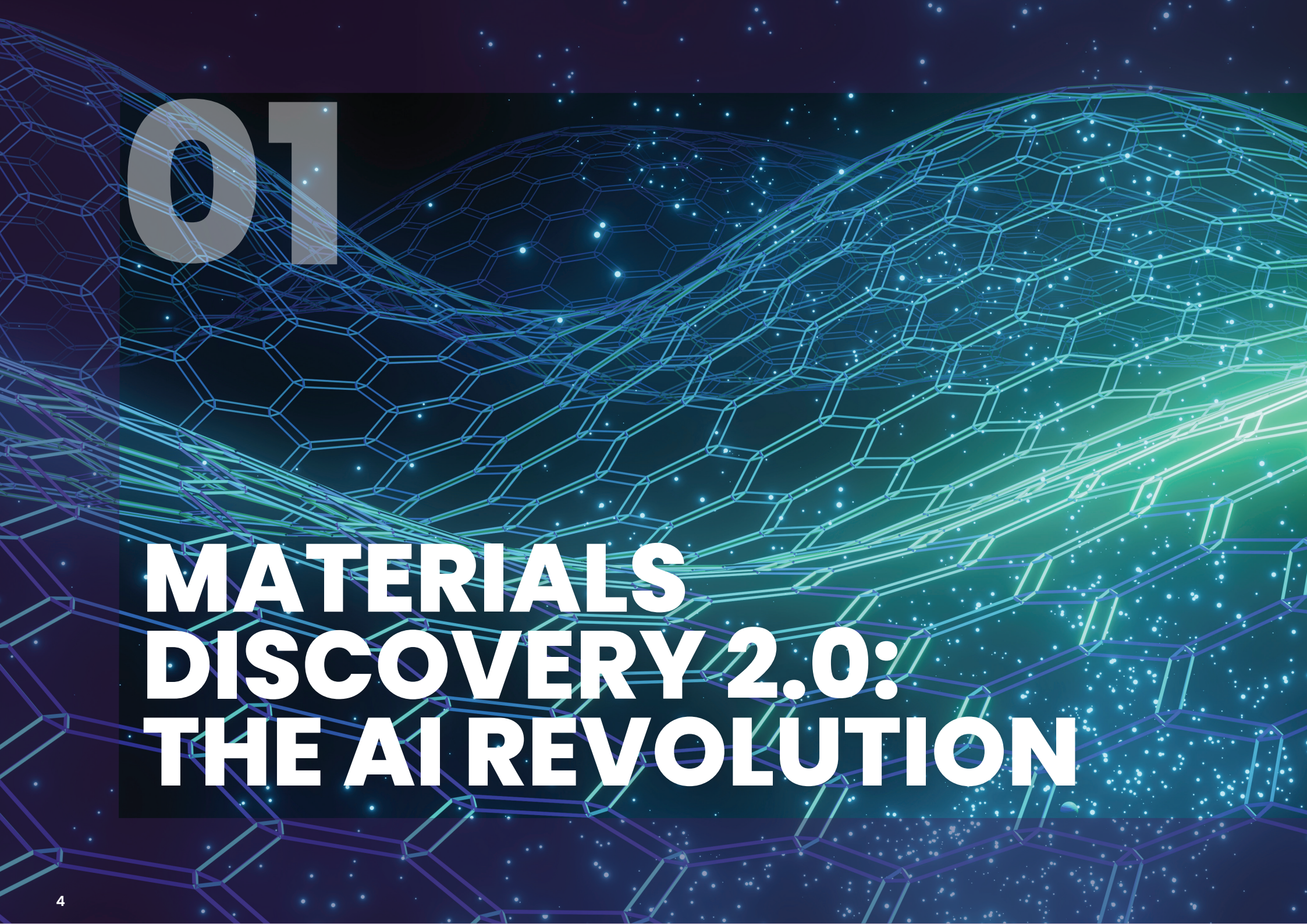
AI-driven materials discovery is not without its challenges:

- **Existing synthesis methods and tools are slow and limited**
- **Data is scarce, noisy, and complex**
- **Multiple scales of interaction make modelling a complicated process**

Possibilities

Innovation in the materials science field could revolutionise many other industries. Novel battery chemistries could vastly improve energy storage, making renewables a stable, 24/7 power source. Re-engineered photovoltaic materials may boost solar efficiency, reducing costs and land use. At the frontier, discovering materials that endure extreme conditions in nuclear reactors could enable safer, cleaner power. AI is accelerating this shift by navigating complex material classes like high-entropy alloys and metal-organic frameworks.

Powered by large, high-quality datasets and grounded in a deep understanding of chemistry and physics, AI is becoming an essential tool in materials discovery.



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MATERIALS DISCOVERY 2.0: THE AI REVOLUTION

Artificial Intelligence (AI) has become deeply embedded in modern life, driving advancements far beyond consumer applications like facial recognition and automated services. Its transformative potential extends across industries and scientific disciplines, accelerating discovery, optimising processes, and unlocking new frontiers in innovation.

Material science, in particular, stands at the brink of a revolution. Traditionally, discovering new materials has been a slow, iterative process, guided by human expertise, intuition, and often sheer serendipity. An example is the accidental discovery of Polytetrafluoroethylene (PTFE), a novel polymer with exceptional chemical resistance and non-stick properties—more commonly known to consumers as Teflon™ which is used in cookware today.

The field is highly complex, with an immense search space of material classes, states, and phase behaviours that challenge conventional approaches. AI is uniquely positioned to tackle this complexity, offering powerful predictive capabilities that can systematically accelerate breakthroughs and change how we design and discover novel materials.

AI ENABLES INVERSE DESIGN: REDEFINING MATERIAL DISCOVERY

At the core of AI-powered materials discovery lies inverse design—a transformative approach that redefines how breakthroughs occur.

Instead of relying on intuition or trial and error, scientists specify desired material properties, and AI models can then predict molecular structures which meet those criteria with increasing precision. This flips the traditional discovery process on its head: AI starts with the end goal, navigating the vast chemical space to uncover unknown structures and properties.

Supported by unprecedented computational power, AI-driven materials discovery is advancing towards an inflection point, with major technology players accelerating progress. Google DeepMind's GNoME demonstrated how graph neural networks can predict new material candidates, expanding the catalogue of stable materials tenfold. Microsoft's MatterGen and MatterSim validated the feasibility of novel material candidates using generative AI methods, while Meta's Open Materials 2024 initiative is driving democratisation through open-source datasets and AI models.

By combining advanced algorithms with well-understood chemistry and physics, AI is poised to create a quantum leap in material science. Machine learning, deep neural networks, and generative AI models can rapidly analyse complex compositional landscapes, proposing novel candidates that might otherwise go unnoticed. When powered with scientifically validated data, AI could enable a closed-loop discovery system—compressing development cycles from years to mere days. Beyond accelerating breakthroughs, this approach optimises multiple parameters simultaneously, unlocking next-generation solutions in energy, computing, and beyond.

FULL POTENTIAL OF RENAISSANCE IN MATERIAL SCIENCE WITH CONVERGENCE OF FRONTIER TECHNOLOGIES

To fully realise its potential, AI must be integrated with other frontier technologies. Quantum computing brings the power of solving the dynamics of complex quantum systems, particularly in regions inaccessible to classical computing, such as quantum dynamics. While this opens up the possibility of understanding the dynamical behaviour of systems—such as how exotic materials like superconductors can conduct electricity with no resistance—it is resource-intensive. The convergence of generative AI, quantum computing, and high-throughput automated synthesis, therefore forms a *Catalytic Discovery Core* for next generation materials discovery.

This harnesses the predictive power of generative AI to propose novel candidates, the computational power of quantum computing to sieve out the most viable candidates, and the fast turnaround of high-throughput automated synthesis for rapid empirical validation. However, the true benefit from the combined use of the three potent techniques lies in the ability of generative AI to learn from real-world data that is generated to improve its predictive performance and reliability.

INVESTING IN THE AI-DRIVEN FUTURE OF MATERIAL SCIENCE AND DISCOVERY

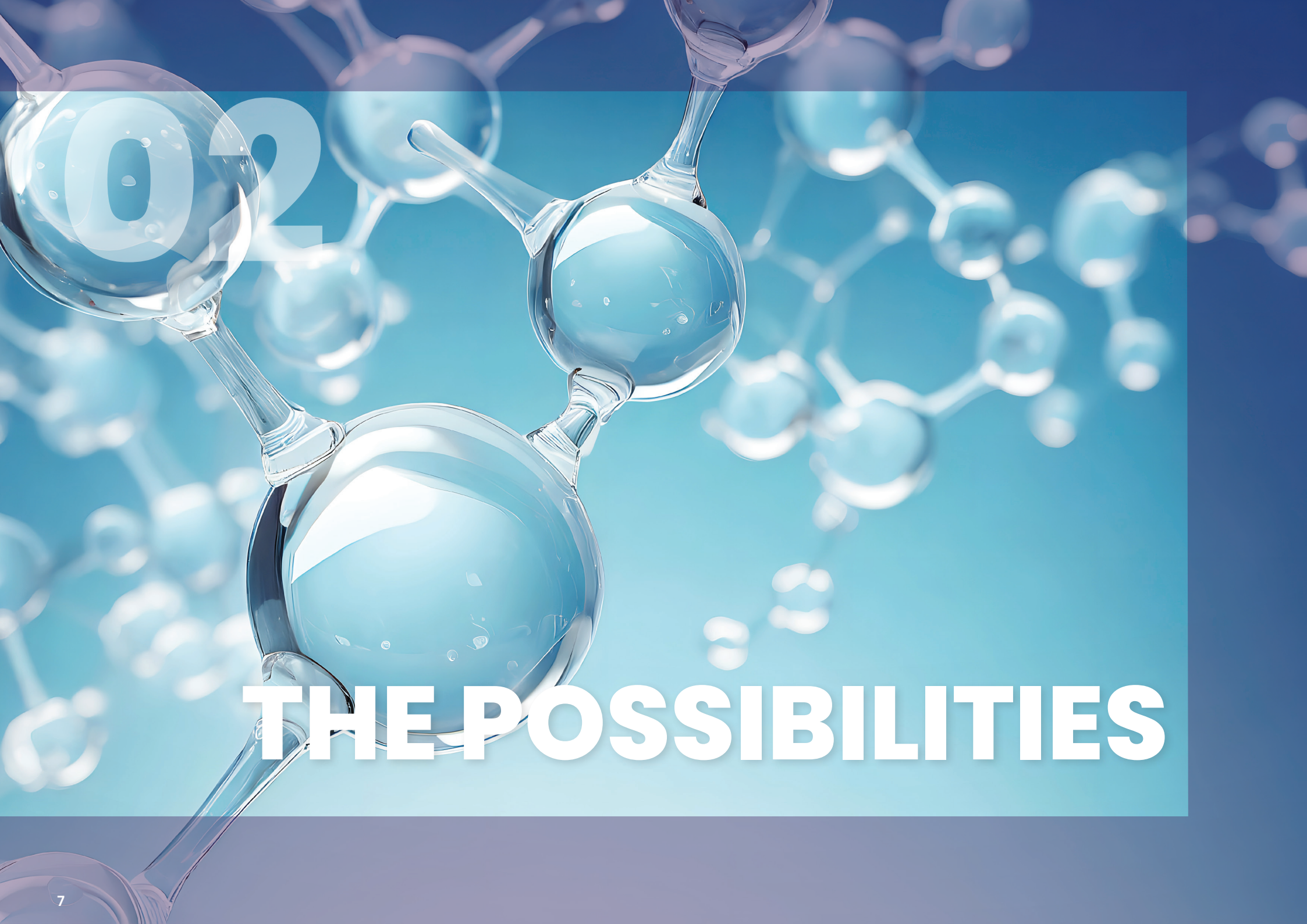
As a generational investor, Temasek seeks to deliver sustainable returns over the long term. Temasek believes that tech-driven innovations can create large future markets that can impact its portfolio. The firm has formed an Emerging Technologies team with the aim of identifying technologies to future-proof its participation in major future market inflections such as AI-driven material science and discovery. In addition to making direct investments in tech-driven innovations, Temasek has formed Xora Innovation, its deep tech investment platform that invests in startups in three key sectors: compute & communications, climate & energy, and AI in physical industries.

“We are witnessing a renaissance in material science, catalysed by the convergence of AI and advanced materials. AI is not just an enabling tool—it is a catalytic force reshaping how materials are discovered, designed, and deployed.

While AI today complements scientific intuition—accelerating discovery by exploring vast material possibilities—quantum computing will become a powerful companion, unlocking levels of precision and complexity beyond what AI alone can achieve.

At Temasek, we actively track such paradigm shifts to position ourselves to support breakthroughs and scale solutions for a more sustainable and resilient future.

Mr Russell Tham
Head, Emerging Technologies, Temasek



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THE POSSIBILITIES

A truly effective AI-driven materials discovery system must function with an adaptive, self-improving closed-loop system, leveraging active learning to enhance accuracy and efficiency. At its core, this system needs to be trained on diverse, high-quality scientifically validated datasets, free from bias and noise, ensuring accurate predictions. Using inverse design, AI could dynamically pinpoint the most promising regions within the vast chemical space, strategically generating novel material candidates with optimised structures and properties.

Thereafter, promising material candidates would be synthesised and characterised in a high-throughput manner, where experimental validation determines their real-world feasibility and performance. Validated data would then be continuously fed back into the AI model—where active learning algorithms prioritise the most valuable new data points to refine predictions. This self-improving feedback loop optimises experimental efficiency, enabling rapid iteration.

However, to deliver meaningful innovation, such a system needs to be scalable—progressing from nanogram-scale synthesis to grams, kilogramme, and ultimately industrial-scale production. A fully integrated closed-loop system would thus significantly accelerate discovery, bridging the gap between computational prediction and real-world application to drive the next generation of advanced materials.

A fully integrated closed-loop system would thus significantly accelerate discovery bridging the gap between computational prediction and real-world application.

“While pharma is leading the pack with AI-based materials discovery, we are seeing AI accelerating materials innovations across batteries, alloys and composites, semiconductors, optics, biomaterials and many others. The sector is still early—but moving at a rapid pace.

Mr Rajesh Swaminathan
Partner, Khosla Ventures

The ideal scenario: A robust AI-enabled materials discovery closed-loop system

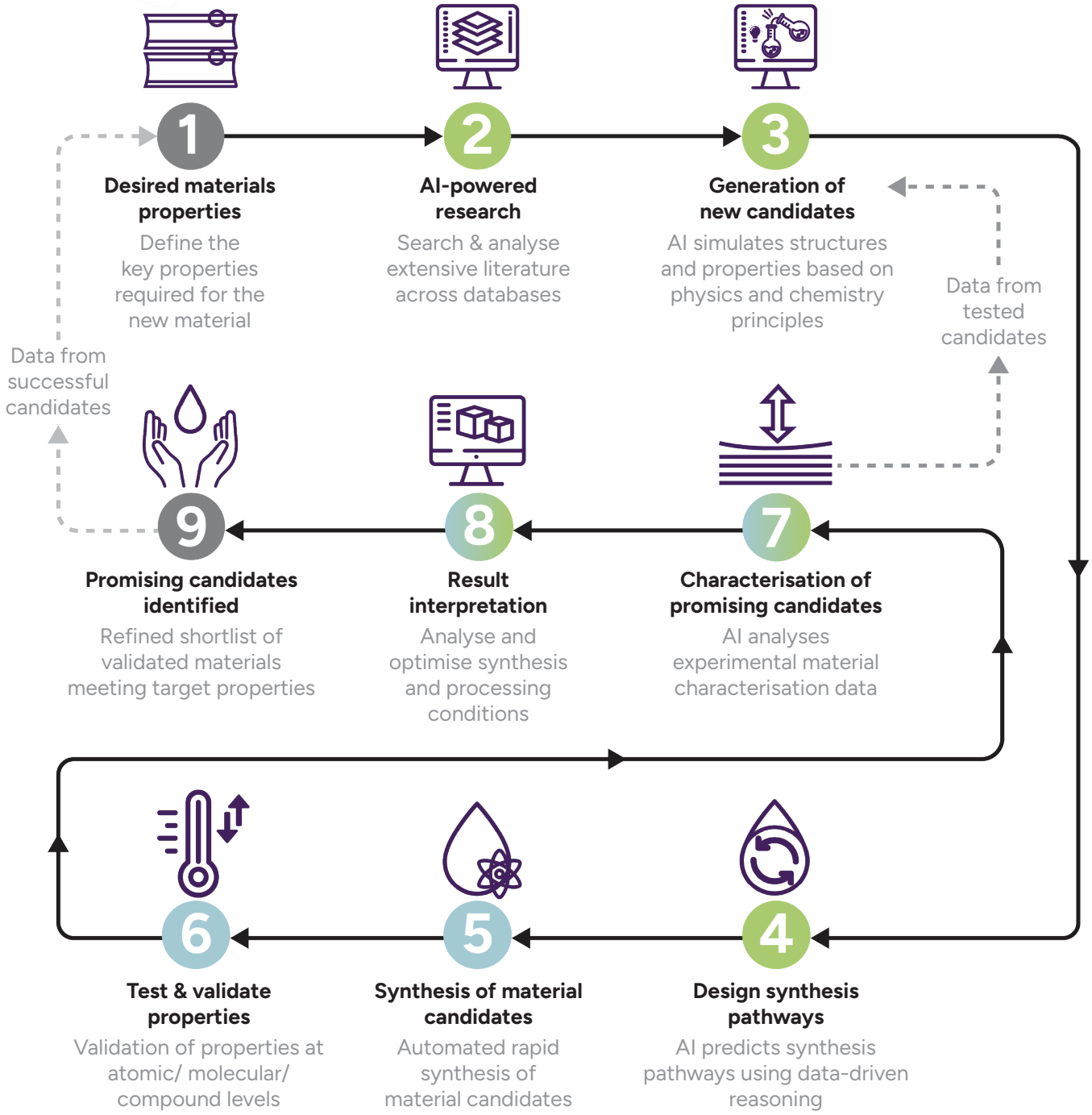
THE PERVASIVE IMPACT OF AI IN MATERIALS DISCOVERY HINGES ON TWO CRITICAL FACTORS:

1. Generative AI models grounded by scientifically validated data

A high-performance AI-driven discovery system must seamlessly integrate generative models with real-world experimental data, operating within a tight feedback loop. This ensures AI predictions are continuously refined through empirical validation, enhancing accuracy and accelerating discovery.

2. Synthesis and testing of materials at scale

The ability to rapidly synthesise and test materials at scale across diverse material classes is fundamental to unlocking AI's full potential in material science. High-throughput experimental platforms could enable the systematic validation of AI-generated candidates, closing the loop between prediction and real-world application.



AI-enabled Human intervention

> **AI is revolutionising materials discovery, but additional toolsets are needed to transform entire energy and industrial systems. By integrating AI with autonomous experimentation, we can co-optimise materials design, manufacturing, and deployment, unlocking scalable pathways for decarbonisation.**

Dr Evelyn N. Wang
Vice President for Climate, MIT

A World of Potential Around the Corner

Beyond AI's ability to rapidly simulate material structures and predict their properties, two key trends are set to amplify its transformative potential:

1. The rise of open-source AI tools is levelling the playing field in materials innovation

Historically, access to advanced computational models and large materials datasets was restricted to well-funded institutions, limiting the speed and scope of innovation. Now, open-source AI is democratising discovery, enabling researchers worldwide to harness sophisticated predictive models at reduced computational costs. As AI models become more computationally efficient and incorporate enhanced reasoning capabilities, designing and development of novel materials could be executed with unprecedented precision and time.

2. As quantum computing matures and converges with AI, the resulting synergy has the potential to exponentially enhance materials discovery

In classical computing, simulation offers a way to bypass traditional synthesis and testing, and the need for expert interpretation of results. Such computational tools rely on efficient algorithms that approximate the quantum mechanical[1] behaviour of electrons and nuclei to predict static properties such as ground state energies and configurations. However, there exist regimes that are beyond the reach of classical computing, such as where material properties

[1] *Refers to the rules that govern how very small particles—like atoms and electrons—behave, often in ways that seem strange compared to everyday physics.*

and behaviour require a dynamical description or systems that exist far from equilibrium. This is because classical computing remains constrained by an inability to capture the correlations of quantum motion and behaviour. Materials with emergent properties such as superconductors[2] and quantum dynamical phenomena such as in chemical reactions and charge-energy transfer are hard to describe without an exponential increase in resources due to the complex interactions among electrons and nuclei. Thus, we see that nature is inherently quantum and is best simulated by a quantum computer that operates on the same quantum mechanical principles as the systems it seeks to simulate.

The convergence of quantum computing and AI therefore unlocks the ability to simulate and design even the most complex materials, particularly where classical computing reaches its limits. It offers the potential to accurately model material properties at the atomic and electronic scale, including those involving complex quantum phenomena. With more refined data, generative AI will improve its predictive abilities and produce even higher quality data in an accelerating cycle.

While still in early stages, rapid advances in quantum hardware, error correction, and hybrid quantum–classical frameworks are making these approaches increasingly viable. The path toward practical quantum-enhanced materials discovery is no longer theoretical—the pace is accelerating. The advent of quantum computing is unstoppable as evidenced by the interest in DARPA's Quantum Benchmarking Initiative and recent announcements by leaders such as Google, IBM, and Microsoft.

"Many of the toughest challenges in semiconductors stem from the limitations of conventional materials and scaling approaches. The convergence of AI and quantum computing opens the door to designing and simulating complex materials—such as superconductors and correlated oxides—that could unlock breakthroughs in next-generation computing architectures."

Dr Sundar Ramamurthy
Former General Manager,
Applied Materials

[2] *Superconductors exhibit zero electrical resistance when cooled to a particular temperature, highly valuable for applications in energy transmission, computing and medical imaging.*

> **AI is a research multiplier in material science, accelerating breakthroughs by leveraging high-throughput experimentation and robust data.**

Prof Loh Xian Jun
Executive Director,
A*STAR, Institute of Materials Research and Engineering

Poised for Innovation

AI is most effective when applied to materials with large, high-quality datasets and well-understood chemistry and physics. These conditions create an ideal landscape for AI to accelerate discovery, optimise compositions, and unlock new functionalities. Two promising material classes that exemplify AI's potential are High-Entropy Alloys (HEAs) and Metal-Organic Frameworks (MOFs).

High-Entropy Alloys

Significance

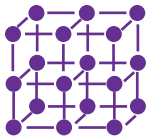
This represents a shift in materials design, offering transformative strength, corrosion resistance, and thermal stability—critical for aerospace, nuclear energy, and high-performance industrial applications where conventional alloys fall short. Unlike traditional alloys, which rely on one or two dominant elements, HEAs incorporate five or more elements in near-equal proportions, creating atomic structures with superior mechanical and thermal properties.

Challenges

However, their vast compositional space presents a major discovery bottleneck. With millions of possible metal combinations, identifying the right alloy through conventional trial-and-error methods is impractical and inefficient.

AI as a Catalyst

This is where AI becomes a game-changer. By leveraging large datasets of elemental properties, it can predict atomic-scale interactions, thereby guiding the discovery of optimised HEAs. Because HEAs are relatively straightforward to synthesise, AI-driven models can accelerate experimental validation, dramatically reducing the time required to develop next-generation alloys tailored for extreme environments.



Metal-Organic Frameworks

Significance

Marking a major advancement in materials science, these structures offer ultra-high porosity, tunable chemistry, and vast surface areas—making them highly versatile for gas storage, carbon capture, and drug delivery. Their modular structure, composed of metal nodes connected by organic linkers, allows for an almost infinite number of configurations, enabling researchers to tailor MOFs for specific applications.

Challenges

But this immense design flexibility also presents a significant challenge. With millions of possible metal-linker combinations, identifying MOFs with optimal properties through traditional trial-and-error methods is slow and resource-intensive.

AI as a Catalyst

AI offers a powerful tool to help navigate this complexity by analysing large datasets of synthesised and predicted MOFs, recognising patterns in atomic structures, and suggesting novel configurations with tailored properties.

Powering the Energy Transition

AI-driven materials discovery is revolutionising next-generation energy solutions, transforming how researchers identify and optimise materials to address critical technological bottlenecks. These advancements come at a critical time as the global energy transition is being shaped by three key forces: escalating climate change, geopolitical risks affecting energy security, and surging global energy demand. Accelerated material innovation through inverse design is essential.

The following examples illustrate how AI is driving breakthroughs in next-generation materials to enable the energy transition.

> **"The rapid progress in large-parameter deep-learning models, autonomous laboratories, and AI systems for reasoning suggests a future of AI-enabled discovery of exceptional new materials—materials with record breaking performance such as near-room temperature superconductors, new catalysts for synthesising sugars, resilient materials for hydrogen storage or first-wall materials for fusion reactors.**

Prof Rajeev Ram
Partner (Ventures),
Breakthrough Energy

Technology	Key Limitations	Unlocking Potential with AI
SOLAR PANELS	Commercial solar panels convert only 15–22% of sunlight into energy, as silicon absorbs a limited range of wavelengths, with excess energy lost as heat.	• By analysing electron band gaps, optical absorption, and carrier mobility, AI is accelerating the optimisation of perovskite-based semiconductors as photovoltaic materials, enhancing their efficiency, stability, and scalability. • This data-driven approach could potentially increase solar cell efficiency to 40% or more, supporting their path to large-scale commercialisation.
NUCLEAR FUSION REACTORS	The extreme conditions inside fusion reactors—temperatures exceeding 1,000°C and intense radiation flux—push materials to their limits, causing structural degradation and reduced performance over time.	• AI can speed up the discovery of radiation-resistant, high-temperature materials by optimising multiple properties at the same time—including thermal stability, mechanical strength, and radiation tolerance.
BATTERIES	Lithium-ion batteries are reaching their energy storage limits, requiring new materials to improve capacity, lifespan, and charging speeds.	• Battery chemistry involves intricate electrochemical processes. Factors like electronic structure, ion transport, and reaction kinetics must be optimised simultaneously. • AI can rapidly analyse millions of potential material combinations, predicting how they will perform across different conditions. This accelerates the discovery of high-performance electrodes and electrolytes.

Example: Cosmos Innovation

Singapore-based startup Cosmos Innovation, backed by leading minds in AI (including Demis Hassabis, the CEO of DeepMind and Nobel Prize Winner 2024) is also using AI to address the challenges of existing silicon-based solar panels which are reaching their fundamental limits in efficiency. Backed by Temasek's investment platform Xora Innovation, it is on a quest to find process recipes for next-gen perovskite silicon tandem solar cells that are most efficient and cost-effective.

"Integrating AI and machine learning into battery materials research is a game-changer. We now have a clear view of the rich literature—how many molecules and materials have been discovered and what properties have been tested in batteries. Generative AI accelerates the discovery of novel materials, to overcome current technological limitations and rapidly advance energy storage solutions.

Dr Shirley Meng
Principal Investigator, Laboratory for Energy Storage and Conversion, University of Chicago

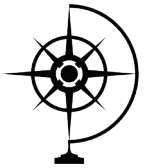
03

THE LANDSCAPE TODAY

> **Integration of AI into material science will help bridge the gap between academic discovery and commercial impact. More specifically, AI used properly will derisk early-stage research and discoveries of cutting-edge materials, accelerate validation in high value products and create scalable pathways in the deployment of the materials technology in general.**

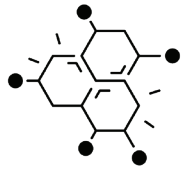
Dr Carmichael Roberts
Co-Founder and Managing Partner, Material Impact

Three Common AI Methods for Materials Discovery



The Navigator:
Graph Neural Network (GNN)
Maps out the complex relationships between different elements at atomic and microstructural levels.
Example: Google's Graph Networks for Materials Exploration (GNoME).

The Painter:
Diffusion Models
Accurately models and visualises molecular structures and reveals defects within materials. It does this by "diffusing" samples with random "noise", before the diffusion is reversed to create an accurate picture of the molecular structure.
Example: Microsoft's MatterGen.



The Mimic:
Generative Adversarial Network (GAN)
Generates new material structures. "Near-real" data is generated before being fed back to the model as a negative example to train it to produce increasingly realistic data.

Given the complexities of material science, virtual simulations and synthetic data generation are not sufficient to address the critical need for experimental data to ground AI models effectively. The field requires a deep integration of computational predictions with real-world experimental validation to ensure accurate and reliable outcomes. We outline some crucial challenges in the next few pages.

1. BEYOND PREDICTION, AI NEEDS VALIDATION

Imperative

While AI can simulate and predict promising material candidates, its accuracy depends on how well its models are grounded in real-world chemistry and physics. Experimental validation is one of the essentials to refine AI predictions, yet existing synthesis methods are often too slow and limited in scale.

Problem

Automated material synthesis solutions currently rely on modifications of existing industry tools, which often fall short in throughput and scalability. These systems are not designed to handle the vast volume of samples required for the rapid screening and synthesis essential to AI-driven discovery.

Possibility

To realise AI's full potential in material science, automated and high-throughput experimental hardware must evolve in parallel with AI capabilities, generating real-world data at a pace that matches the rapid output of computational models. A synchronised closed-loop system—where AI predictions and empirical validation operate seamlessly—remains a critical missing link.

In contrast, other fields, such as drug discovery, have successfully adopted high-throughput workflows, screening samples at exponentially higher rates. The challenge in material science is more complex: working with solid-state materials requires specialised solutions, including multi-stage processing (mixing, grinding, and pressing), along with contamination control strategies. Without advancements in synthesis automation, AI-driven materials discovery will remain constrained by experimental bottlenecks.

While synthetic data cannot replace real experimental validation, emerging approaches such as expert guided training of AI models using physics-based rules has proven valuable in other fields such as the modelling of thermal conduction in integrated circuit design. This approach could help enhance AI-driven materials discovery by improving predictive accuracy, bridging data gaps, and accelerating the identification of novel materials.

A synchronised closed-loop system—where AI predictions and empirical validation operate seamlessly—remains a critical missing link.

High-quality experimental data for emerging materials is severely limited—creating a persistent bottleneck in the AI-driven discovery pipeline.

2. DATA CHALLENGES: SCARCE, NOISY, COMPLEX

Imperative

AI-driven materials discovery is fundamentally constrained by data availability, quality, and complexity. While well-documented datasets exist for basic elements and conventional compounds, data on novel and non-conventional materials—such as superconductors—remain scarce. Furthermore, existing datasets are often inconsistent, biased, or noisy, further complicating training of AI models.

Problem

A key challenge is the heterogeneous nature of material science data, which exists in diverse formats—ranging from graphs and spectroscopic readings to microscopy images—making standardisation and large-scale analysis difficult. In addition, current AI foundation models are often too generalised for the specialised needs of material science, lacking the specificity needed for high-precision predictions. The absence of standardisation across experimental techniques further exacerbates data inconsistency, while the limited availability of high-quality experimental data for emerging materials remains a persistent bottleneck in the AI-driven discovery pipeline.

Possibility

For AI to unlock its full potential in this domain, vast quantities of high-quality, standardised data are required, spanning multiple dimensions such as composition, structure, and properties. This necessitates specialised AI models tailored to different material classes, along with substantial computational resources for high-fidelity simulations and active learning-driven optimisation.

A promising approach is the development of small domain-specific foundation models that focus on targeted problem spaces rather than a single, multimodal AI model attempting to generalise across all material types. This would help address both cost and efficiency concerns—as building a large foundation model is expensive but does not inherently create value unless applied to real-world material discovery.

Ultimately, commercial success in AI-driven materials discovery will depend on the value of the materials uncovered. The key question is not just how a material was discovered, but rather why it is better. The true validation of AI-driven platforms will come from the real-world performance and market adoption of the materials they help create—reinforcing the need for focused AI models, robust validation processes, and clear pathways to commercialisation.

3. MODELLING COMPLEX CHEMICAL INTERACTIONS

Imperative

Materials discovery is rooted in understanding how compounds are formed from basic elements and how they behave under varying conditions. However, the field is inherently complex due to intricate chemical interactions influenced by multiple variables—including temperature, pressure, and composition ratios—all of which must be precisely controlled to achieve desired material properties. Compounding this challenge, material science involves high-dimensional data, where a vast number of interdependent factors dictate performance, making both predictive modelling and experimental validation exceptionally difficult.

Problem

AI models struggle to integrate multiple scales of interaction—from quantum mechanical effects at the atomic level to macroscopic material properties. In addition, AI systems face difficulties in balancing thermodynamic stability and reaction kinetics—a critical factor in materials synthesis. The lack of standardised data formats and inconsistencies in experimental measurements further hinder AI's ability to generalise across diverse materials, posing a fundamental roadblock in AI-driven materials discovery.

Possibility

AI models for material science must be capable of simultaneously modelling reaction kinetics and thermodynamics to accurately capture complex chemical behaviours. Additionally, AI systems must be designed to process high-dimensional datasets efficiently, identifying optimal synthesis pathways that balance multiple interacting variables. Advancing these capabilities will be critical to enabling AI-driven breakthroughs in materials discovery.

While these challenges are significant, by addressing limitations in data quality, synthesis scalability, and complex chemical modelling, AI could enable a generational leap in materials innovation—one that reshapes energy, computing, and manufacturing, driving progress at an unprecedented pace.

AI must bridge the gap between atomic-scale theory and real-world synthesis to drive meaningful breakthroughs in materials discovery.

A New Era

Technological revolutions often begin with subtle, incremental progress—small shifts that seem almost imperceptible. But as breakthroughs accumulate, transformation often happens all at once.

AI-driven materials discovery, while still in its early stages, is gaining momentum. The field is approaching an inflection point, driven by advances in generative AI models trained on increasingly large, high-quality experimental datasets across diverse material classes.

Complementing these advances, the continued maturation of quantum computing and high-throughput automated synthesis will expand what is possible in simulation and validation, laying the groundwork for deeper synergy over time. Manufacturers, who have embraced the use of AI, are also working on quantum algorithms in preparation for the arrival of quantum computing. Together, these technologies form a *Catalytic Discovery Core* for next generation materials discovery, helping to bridge the longstanding gap between computational design and empirical validation, enabling more rapid and scalable materials innovation.

These advances would translate into real-world impact, with potential applications across industries—from next-generation textiles that adapt to extreme environments, to ultra-lightweight alloys with extraordinary strength, and entirely new material classes with emergent properties.

AI is not just accelerating discovery—it is reshaping the foundation of how we design and engineer materials. And as complementary technologies continue to mature, they will further amplify AI's ability to define the next frontier of material science.

"Science thrives on bold questions and relentless curiosity. In this transformative era, we transcend boundaries—merging insight with innovation to uncover materials that redefine our understanding of possibility and progress.

The use of AI for materials design opens new opportunities to create dynamic materials, which can adapt to changes in the immediate environment. Furthermore, it will streamline the production of such materials, as it incorporates the materials synthesis into the design process.

Nobel Laureate,
Prof Sir Konstantin 'Kostya' Novoselov
Tan Chin Tuan Centennial Professor
National University of Singapore

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Authors

Prof Alfred Huan
Corporate Advisor, Emerging Technologies, Temasek

Dr Daniel Tay
Vice President, Emerging Technologies, Temasek

Ms Jingxi Yew
Vice President, Emerging Technologies, Temasek

With special thanks to

Dr Joel Leong
Director, Xora Innovation

Dr Dickson Thian
Vice President, Xora Innovation

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