



The next phase of materials discovery

New technologies are already changing the field. When we put them together, they'll change everything.

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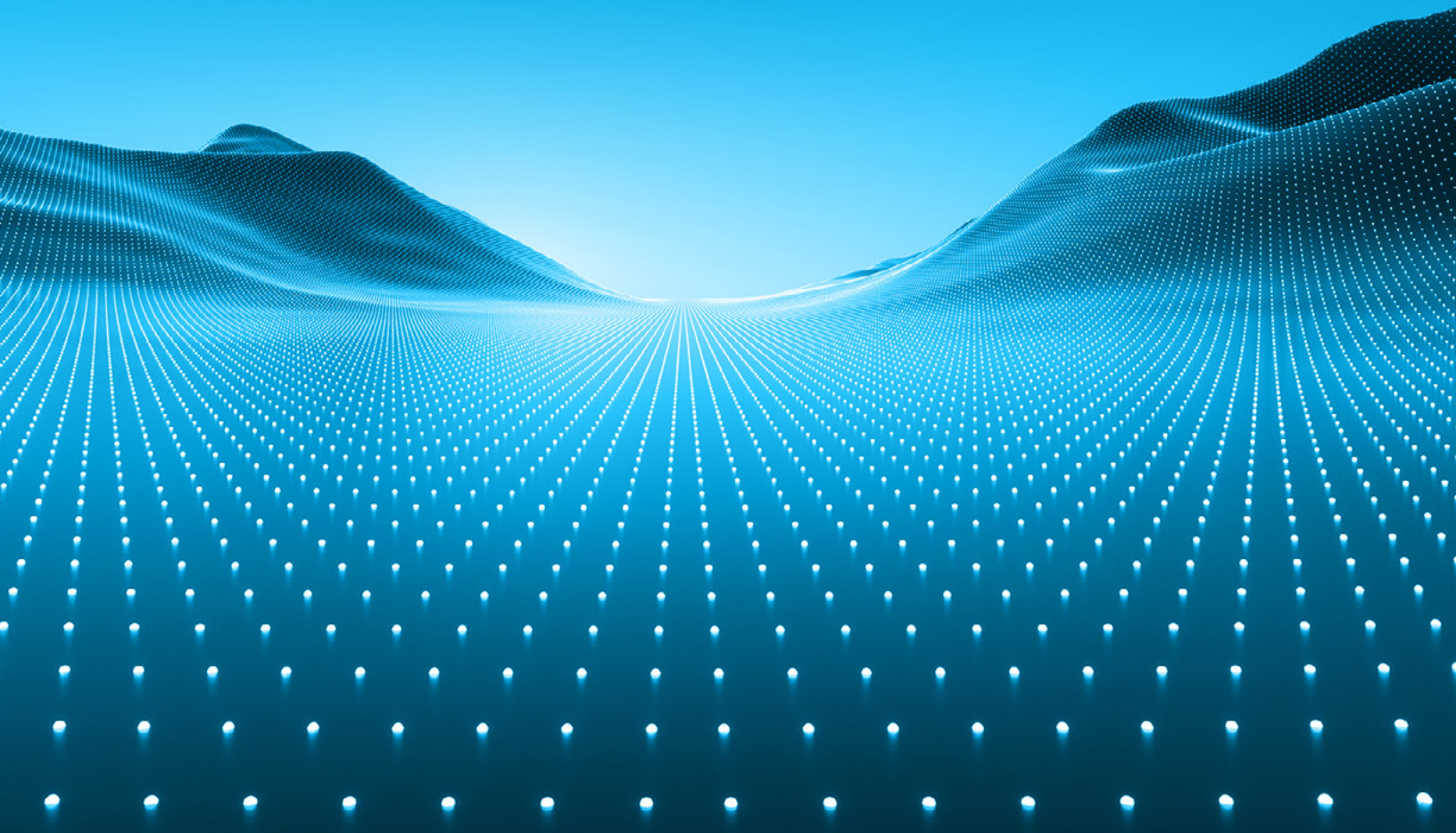
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A new age of discovery



Materials are so central to human civilization that they define our history. The stone age. The copper age. The bronze age. Anything before the iron age feels foreign to us, while our achievements here in the silicon age would look like magic (or witchcraft?) to our ancestors. From the use of flint and steel to create fire to the use of semiconductors to create transistors, advances in materials consistently drive innovation. Without the right materials, no technology would exist.

For decades, materials science operated as a downstream function of engineering. Today, it has moved to the absolute top of the strategic corporate and geopolitical agenda. This shift is driven by a powerful convergence: an explosion in demand for new materials, and an unprecedented ability to supply them.

This paper focuses on the discovery of novel materials, and the potential for another great leap forward. It draws on a recently published perspective developed with partners from industry, academia and national laboratories (government-funded and private research laboratories and large-scale user facilities), and translates those insights for a broader industrial audience.

Computing is reshaping materials science in many ways, from advances in computational modelling and AI-driven discovery to the emerging role of

quantum computing. But despite revolutionary advances in technology, many of the processes underlying materials research lag behind. The time has come to challenge traditional processes. Above all, this means breaking down the boundaries between the various disciplines within materials discovery.

Beyond their individual contributions, the greatest advances will come through increased collaboration between these fields. This paper closes with a collaboration roadmap for each discipline, examples of successful collaboration, and the potential for an age of unprecedented materials innovation.

Most promising materials never reach deployment. Not because they lack performance, but because manufacturability, supply-chain constraints, degradation behavior and real-world operating conditions arrive too late in the discovery process.

1. We use “national labs” as a shorthand for public and private laboratories that conduct research in the public interest.

The valley of death



The path from concept to real-world industrial application remains one of the most formidable challenges in materials science. The gap between them even has a name in the industry: “the valley of death.” Researchers may devote years or even decades to developing a new material, based on a promising model. This represents not only a scientific hurdle, but an economic and strategic one as well. Pulling the plug too early could result in missing a breakthrough material, while waiting raises the risk of late-stage failures.

Over the last two decades, the search for new materials has accelerated dramatically, thanks to the field of computational material discovery, which uses advanced computing to identify promising materials. But there’s a problem with the way most labs use this approach, and it’s making the “valley of death” wider, right when we should be working to narrow it. We have the technology to shrink this gap. What we’re missing is a well thought-out strategy on how to use that technology.

New technologies call for a new workflow

Industry demands materials that are not just innovative but manufacturable, stable, and economically viable. This creates what we call the “robust optimization challenge” – finding materials that perform well not just under ideal conditions, but across the messy realities of production and use.

The aerospace industry exemplifies this challenge perfectly. As engine efficiency requirements drive operating temperatures ever higher, the theoretical properties of candidate materials become secondary to their stability under extreme thermal cycling, resistance to oxidation, and compatibility with existing manufacturing processes. Similar challenges emerge in energy storage, where promising battery materials often falter when confronted with the realities of mass production and long-term cycling stability.

However, despite the importance of robustness, researchers often wait until surprisingly late in the discovery process to check for it. In the theory stage, we’re only looking for one or more unique qualities, but then in the physical testing phase we also expect that material to stand up to extreme conditions. Taking a new material from vision to reality is hard enough. When we wait until the end to test for robustness, we’re also changing the criteria halfway through.

Many discovery pipelines still operate as if computation, synthesis, characterization, processing, and scale-up existed in a sequence rather than a connected loop. In practice, every stage influences every other, and the workflow should reflect that. The early phases of discovery must include the same criteria as the end phases. Processing windows, environmental limits, degradation mechanisms, lifetime constraints, and regulatory considerations all need to appear much earlier in the computational landscape.

This is a prime example of the value of merging disciplines. From the outside looking in, it feels obvious that that we should search for materials that may actually work from the start. But this won’t happen unless a team decides to make it happen.

Consider a computational analyst tasked with identifying a certain material. It would be unusual to stop and ask how the material will be manufactured, what regulations it might face, or how it could degrade after years of use. In fact, at this phase it’s possible that no one has considered these factors. The challenge is not a failure of individual researchers, but a workflow that has yet to connect the pieces. The fact that a more integrated approach makes sense does not make it inevitable. It must be designed into the way teams work.

Integrating the four paradigms of scientific research



Science is usually looked at in terms of progress – advancing from one stage to the next.

This is what John Gray presents with his concept of the Fourth Paradigm, in which **scientific discovery progresses through four approaches: beginning with empirical observation, then moving on to theoretical modeling, computational simulation, and finally data-driven discovery.** Together, these four paradigms represent the complete scientific toolkit that humans use to understand the world around us.

Our claim is that the greatest breakthroughs are achieved when these four paradigms are not treated as sequential, but are combined into one connected workflow.

What we've observed across numerous materials challenges is that breakthrough innovations rarely emerge from any single paradigm in isolation. Rather, the most transformative advances occur at the interfaces between these approaches where three things happen:

- theoretical insights guide experimental design
- unexpected experimental results challenge computational models
- data analysis reveals patterns that neither theory nor isolated experiments could uncover.

Consider the development of modern battery materials. Progress hasn't come from empirical testing, theoretical models, large-scale simulations, or data mining in isolation. Instead, it has emerged from the creative tension between these approaches. Density functional theory calculations suggest promising cathode

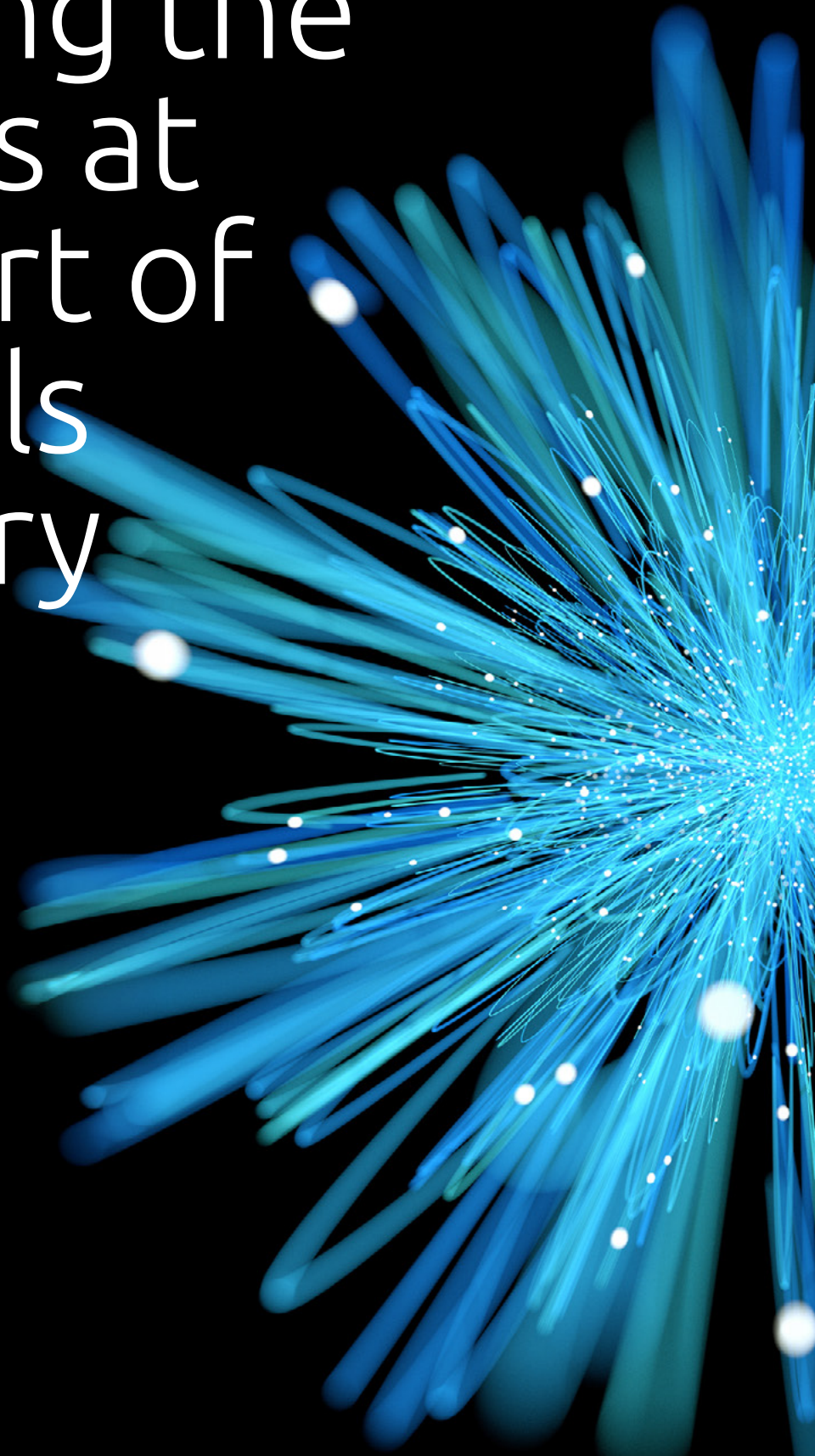
compositions; high-throughput experiments validate and refine these predictions, and machine learning algorithms identify patterns across thousands of charge-discharge cycles to optimize performance. Each paradigm addresses limitations in the others, creating a more robust discovery ecosystem.

We believe we're witnessing the emergence of what might be called "The Great Integration," a fundamentally new approach where the boundaries between traditional scientific methods become increasingly permeable.

This is about developing frameworks where different approaches inform each other continuously, creating a discovery ecosystem greater than the sum of its parts. Now let's go back to the field of materials discovery, and see this paradigm integration in action.



Revealing the
patterns at
the heart of
materials
discovery



The materials search space is simultaneously vast and structured. **With countless possible combinations of elements, structures, and processing routes, exhaustive exploration is impossible. Thus, we rely on patterns to guide us.** This makes intelligent navigation possible, but enormously challenging. And it's what makes the right computational tools and conceptual frameworks so essential.

This challenge is particularly acute in the early stages of materials discovery, where decisions about which compositional spaces to explore can determine the success or failure of entire research programs. Traditional approaches relied heavily on chemical intuition and historical precedent, which often had the effect of constraining exploration to variations on known materials. While valuable, this approach inherently limits the discovery of truly novel materials that might exist in unexplored regions of the compositional landscape.

Computational methods transform the way we navigate this search space by identifying the underlying patterns. These “materials genomes” organize seemingly disparate materials into families with predictable behaviors, changing how we approach the discovery process.

Perhaps the most significant shift has been the development of inverse design approaches. **Instead of starting with a composition and predicting properties, these methods start with desired properties and work backwards to identify promising compositions.** This fundamentally changes the discovery paradigm, much as genome sequencing transformed biology from observation-based to information-driven science. The question becomes not “what properties does this material have?” but “which materials might have these properties?” We’ve found that computational methods help

overcome cognitive biases that have historically limited materials discovery. Human researchers naturally focus on familiar material systems and compositions, while computational approaches can identify promising candidates in unexplored regions of the materials space. This complements human intuition by revealing blind spots and unexpected connections.

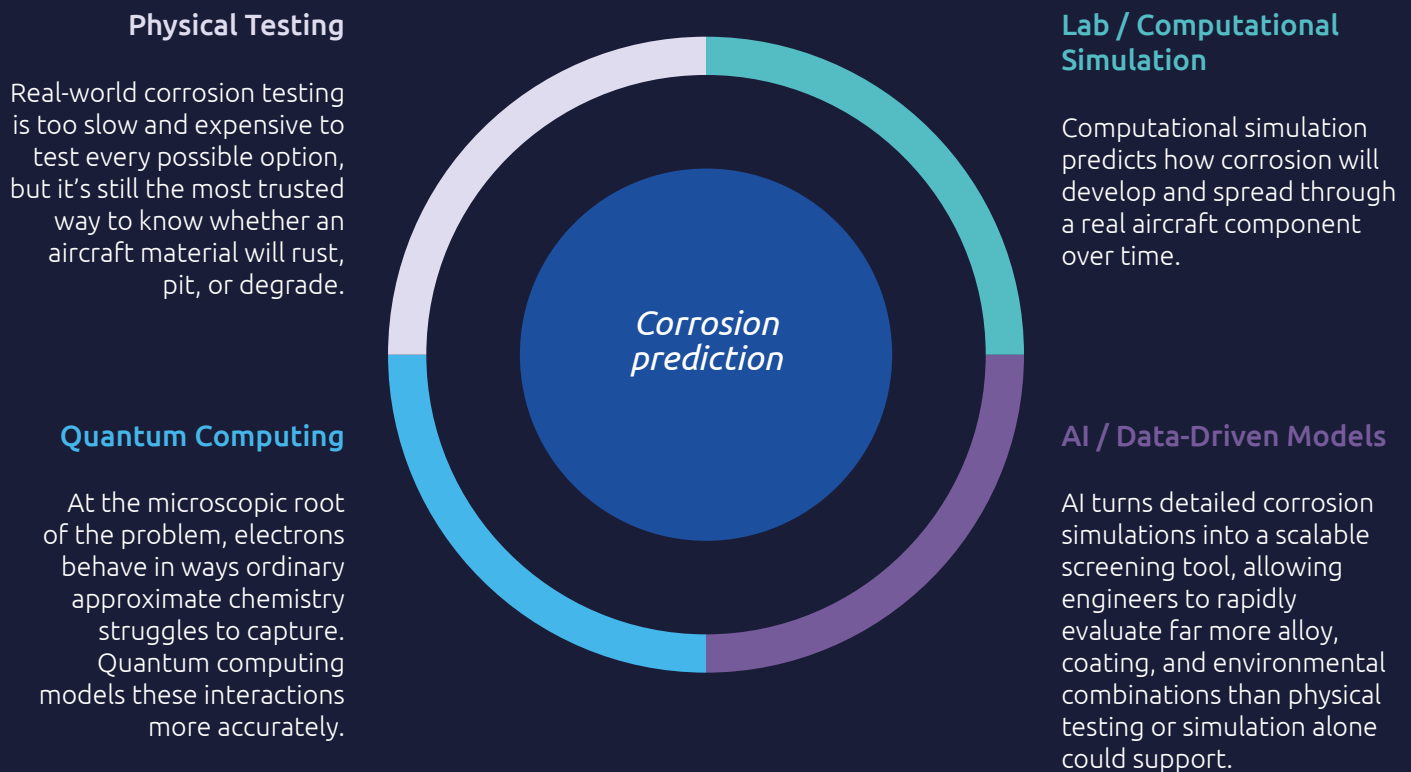
Yet these predictions gain value only when they are connected to observation. Computational simulation can rapidly identify promising regions of the search space, but empirical investigation remains essential for validating results and uncovering unexpected phenomena. Once again, progress is the result of two paradigms merging: empirical observation and computational simulation.



In practice: predicting aircraft corrosion before it starts

Every aircraft that leaves the ground carries a quiet wager: that the alloys holding it together will not surprise the engineers who qualified them. Corrosion is one of materials science's oldest and most expensive problems. Now imagine a different starting point: an aircraft designed with a digital immune system, one that has already identified, atom by atom, exactly where and when corrosion will appear.

That capability is not science fiction. It is being assembled today, thanks to a convergence of physical testing, simulation, quantum computing and AI.



No single technology solves the corrosion problem. Quantum computing improves the chemistry, simulation predicts the engineering consequences, AI expands the search space, and physical testing grounds everything in reality. Together, they create a feedback loop that makes corrosion progressively more predictable.

The evidence base

Aguiar Hualde, J.M. et al. (2025). Quantum Computing in Corrosion Modeling: Bridging Research and Industry, developed with Airbus Central Research & Technology. [arXiv:2412.07933](https://arxiv.org/abs/2412.07933)

See also the companion multiscale-modelling case study (Section 6, this PoV's parent paper) for the underlying active-space and resource-estimation detail.

An abstract digital graphic featuring a dense field of blue dots and lines that form a swirling, tunnel-like structure. A prominent, dark, irregular void is located in the center of the composition, creating a sense of depth and movement. The overall color palette is a range of blues, from deep navy to bright cyan, set against a black background.

New
computation
strategies: doing
more with more

The advances in computational methods extend far beyond computational power. Equally important is how we use that computation. Whereas earlier tools were only capable of isolated calculations of specific properties, today's tools are able to capture the complexity of real-world materials behavior in a wide range of conditions.

Density Functional Theory (DFT) remains the workhorse of computational materials science, but its application has transformed dramatically. Specialized functionals like the Strongly Constrained and Appropriately Normed (SCAN) approach make it possible to simulate materials more realistically, without prohibitive computational costs. This makes accurate, high-throughput screening feasible – a critical capability for accelerating the early stages of materials discovery.

Are we approaching a “completeness threshold”?

It's a tantalizing thought, which would mean that further refinements in computational chemistry yield diminishing returns for materials discovery.

For many properties and material classes, the answer may be yes, suggesting that our focus should shift from incrementally improving accuracy to extracting more insight from existing approaches and applying them to previously intractable problems.

Perhaps the most valuable recent advancement isn't better prediction but better uncertainty quantification – not just calculating a property value, but providing confidence intervals and identifying potential sources of error. This represents a maturation of the field from simply generating predictions to providing decision-relevant information for materials development. Knowing when we can trust computational predictions, and more importantly when we cannot, is often more valuable than marginal improvements in accuracy.

One of the earliest practical uses of uncertainty quantification was deciding what experiment to run next. For example, an AI model might predict that Material A will be 10% harder than Material B, but there's 20% more uncertainty. A scientist-in-the-loop could use these confidence estimates to decide which candidate is worth prioritizing. In this way, uncertainty became a guide not only to what the model predicted, but also to where the next experiment could provide the greatest value.

Another important development is the use of multi-scale modeling approaches, which bridge the gap between atomic-scale simulations and macroscopic properties. By linking methods that operate at different length and time scales, from electronic structure calculations to molecular dynamics to continuum models, we can now trace how atomic-level phenomena manifest in real-world material performance. This capability is particularly crucial for complex materials where different properties emerge at different scales.

The future of computational materials science lies not just in more accurate or faster calculations but in more comprehensive modeling frameworks that capture the complexity of real-world materials behavior. By developing methods that bridge scales, quantify uncertainty, and focus computational resources where they add the most value, we'll be able to make better predictions at lower cost and with fewer experiments.

The background is a dark, almost black, space filled with intricate, glowing patterns. On the right side, there is a dense, wavy structure of bright blue particles, resembling a nebula or a complex data visualization. A prominent, bright orange-yellow trail of particles curves from the top center towards the bottom left, creating a sense of movement and depth. The overall effect is one of high-tech, futuristic, or scientific exploration.

How AI changes the field

AI introduces a new dimension to materials discovery. Unlike theoretical models and physics-based simulations that begin with first principles, AI identifies patterns and relationships directly from data. In doing so, it strengthens the connection between data-driven discovery and the other three paradigms of modern science: empirical observation, theoretical modeling and computational simulation. Rather than replacing existing approaches, AI helps translate insights from one paradigm into another, revealing opportunities that might otherwise remain hidden.

AI also helps identify unexpected relationships between structure and function that might elude human researchers. And this leads to its most transformative potential: the ability of AI to recognize patterns across vast and heterogeneous datasets, revealing design principles that transcend specific material classes or applications.

Rather than simply screening existing compositions, Gen AI can propose entirely new material classes that human intuition might not conceive. Recent work with generative adversarial networks and variational autoencoders has demonstrated the ability to design novel alloy compositions, polymer structures, and even crystal lattices with tailored properties, expanding the materials search space in ways that traditional approaches cannot.

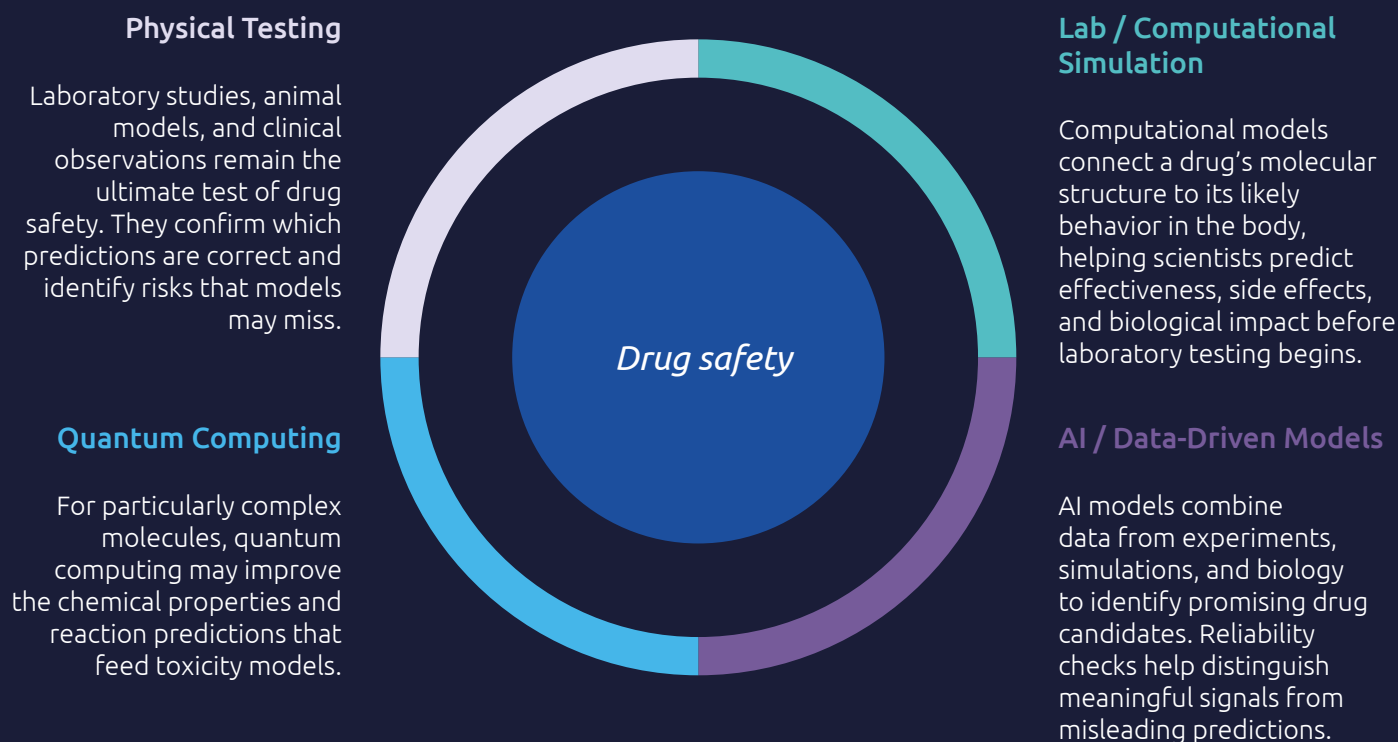
Taken together, these capabilities allow AI to act as a bridge between paradigms. Experimental observations generate data, computational simulations provide additional evidence, and theoretical understanding helps guide interpretation. AI can draw insights across all three, identifying connections that would be difficult to uncover within any single approach.

What about the common “black box” critique of AI in scientific applications? On a positive note, modern explainable AI approaches can actually enhance scientific understanding rather than obscure it. When properly implemented, these methods don’t just predict outcomes but help identify the underlying physical principles driving those outcomes, serving as partners in scientific discovery.



In practice: identifying drug toxicity sooner

A promising molecule can meet its target and still fail because its effects elsewhere in the body are discovered too late. Toxicity is difficult to predict because it emerges across scales: from electronic structure and molecular transformations to protein interactions, cellular pathways, organs, and patient populations. What if discovery teams could identify safety liabilities before costly development?



Together, these technologies solve a challenge that no single approach could manage on its own. Simulations model biological behavior, quantum computing improves key molecular calculations, AI identifies patterns and potential risks, and physical testing validates the results. Once combined, they create a continuously improving system for identifying toxicity earlier in the discovery process.

The evidence base

Early evidence pool: Montgomery, T.W.A. et al. (2023). Data-driven reactivity prediction of targeted covalent inhibitors using computed quantum features for drug discovery, developed with GSK. arXiv:2307.09671

A related hardware study is Kowalik, M. et al. (2026), Executing Utility-Scale Hamiltonian Dynamics for Covalent Inhibitor Reactivity on Quantum Hardware, accepted for QCE 2026, arXiv:2412.15804. These studies illustrate one possible source of quantum-derived molecular features; the broader vignette concerns multi-scale, validated toxicity prediction rather than a specific warhead class or reactivity endpoint.



Data is the
lifeblood of
discovery

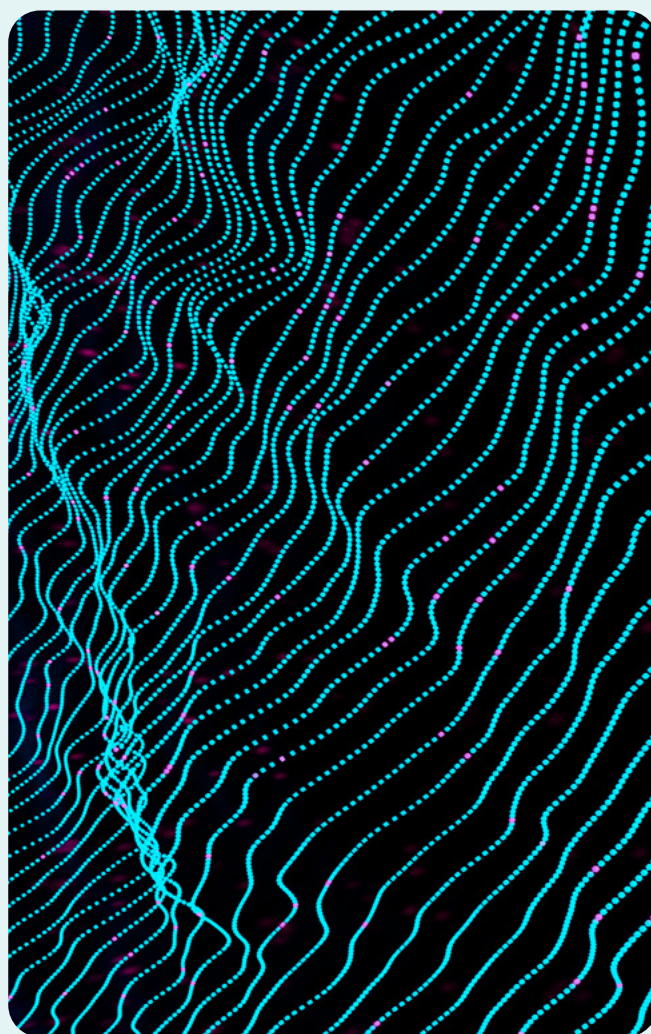
The breakthrough that made AI-driven discovery possible was data sharing at scale. For the entire history of materials discovery until the last two decades, priceless data accumulated in silos. The missing piece to one researcher's puzzle might be sitting in a colleague's file cabinet just steps away, and unless they happened to be discussing their challenges they might never make the connection. The FAIR principles – making materials data Findable, Accessible, Interoperable, and Reusable – underlie one of the greatest changes in materials discovery in our lifetime.

Thanks to the launch of initiatives like [NIMS Matnavi](#), the [Materials Genome Initiative \(MGI\)](#), the [Materials Project](#), and [NOMAD](#), materials science transitioned from isolated experimentation to a connected, data-driven era – the fourth paradigm that we discussed earlier. For the first time, researchers around the world could tap into shared, standardized datasets to help explore AI, machine learning, and high-throughput simulations. Much like the Human Genome Project did for biology, these initiatives laid the foundation for a new paradigm of exploration in materials science with the aim of drastically reducing the time and cost of discovering and deploying advanced materials across industries.

As AI and machine learning continue to mature, their integration with physics-based models and experimental techniques will accelerate. The future lies not in AI replacing traditional approaches, but in deepening the integration of the four paradigms of scientific discovery. Empirical observation generates data, theoretical models explain underlying mechanisms, computational simulations explore possibilities beyond experiment, and AI identifies patterns that connect them all. Together, these approaches create a

self-reinforcing discovery cycle in which each paradigm strengthens the others, accelerating materials innovation far beyond what any one could achieve independently.

For industry, the challenge is not whether data sharing is valuable, but how to do so while protecting intellectual property. Future progress will depend on trusted mechanisms for sharing benchmark data, metadata, failure modes and pre-competitive information without exposing commercially sensitive assets.



Physical
experimentation
plays a
new role



The relationship between computation and empirical observation is becoming increasingly intertwined, with each informing and strengthening the other. Computational models can identify promising directions for investigation, while experiments validate predictions, reveal unexpected phenomena, and generate the data needed to refine future models. **As a result, the role of experimentation is evolving from primary discovery to validation, boundary exploration, and providing training data for computational models.** It is particularly important in capturing the complex, real-world behaviors that computational methods currently struggle to predict accurately.

A counterintuitive insight we've observed across multiple material systems: sometimes deliberately imperfect samples teach us more than perfect ones. When a computational model predicts certain properties for an ideal material, testing that prediction on samples with controlled defects or variations can reveal the robustness of the underlying theory and identify previously unrecognized factors that affect performance. This approach has proven particularly valuable in understanding how defects and microstructure influence properties in functional materials.

For example, a battery material may demonstrate exceptional energy density in simulations and laboratory tests, yet fail to achieve its expected cycle life because small amounts of structural disorder introduced during manufacturing fundamentally alter its degradation pathways. Investigating these imperfections often teaches researchers more about real-world performance

than studying idealized materials alone. The most valuable experiments are increasingly those that produce surprising results – outcomes that computational methods failed to predict. These “productive failures” often reveal limitations in current models and drive theoretical advancement. This perspective suggests that experiments should sometimes be designed to deliberately probe the boundaries of computational predictability rather than simply confirming expected results.

To bridge the gap between computational predictions and experimental reality, one more element is crucial. Computational modeling predicts how a material should look and behave.

In the physical testing phase, we now need to verify how that material actually performs. This is called “characterization.” Techniques like atom probe tomography, aberration-corrected electron microscopy, and synchrotron-based spectroscopies provide atomic-level insights into material structure and behavior, creating direct verification of the predictions posed by computational models at the smallest scales.

We envision a future where automated, AI-guided experimental platforms work in closed-loop systems with computational models – automatically generating data, updating models, and designing new experiments without human intervention. Early examples of such systems are already emerging in areas like battery materials development and catalyst discovery, pointing toward a new paradigm where the boundary between computation and experimentation becomes increasingly fluid.

Unlocking the potential of quantum computing



Quantum computing is often presented as the next great revolution in materials science. In reality, its near-term impact is likely to be more subtle, but potentially quite valuable. The most promising opportunities come from combining classical and quantum approaches in ways that allow each to solve the problems they are best suited to address.

This distinction matters because many of the most important challenges in materials science are fundamentally quantum mechanical. The behavior of electrons determines how materials conduct electricity, store energy, catalyze chemical reactions, and respond to magnetic fields. While classical computing has enabled extraordinary advances in our ability to model these phenomena, some problems remain stubbornly difficult because the quantum interactions become too complex to simulate efficiently.

One of the most promising targets is a class of materials known as strongly correlated systems. In these materials, electrons cannot be treated independently because the behavior of each electron is strongly influenced by many others. This collective behavior produces properties that classical methods struggle to model accurately. Strongly correlated materials – including transition metal compounds, high-temperature superconductors, and complex magnetic materials – therefore represent some of the most compelling opportunities for future quantum approaches.

These materials matter because they sit at the heart of some of the most important challenges in modern materials science, including advanced batteries, superconductivity, magnetic materials, and next-generation electronic devices.

Even modest improvements in simulating these areas could significantly reduce uncertainty.

What would a workflow combining traditional and quantum computing look like? Let's take the example of a new material for batteries. Classical computing might suffice for the material in general, while quantum resources could focus on critical regions, such as the interfaces where lithium ions move between materials and complex electron interactions occur. Researchers can thus target quantum computing for areas where it provides unique value. This hybrid approach is emerging in architectures such as quantum-centric supercomputing, where quantum processing units work alongside traditional high-performance computing systems.

Beyond hardware integration, algorithmic innovations at the quantum-classical interface represent a particularly promising frontier. Approaches such as quantum-enhanced optimization, quantum machine learning, and quantum embedding methods aim to combine the strengths of both computational paradigms. Long before fully quantum approaches become viable, these hybrid methods may begin delivering practical benefits for materials discovery.

Quantum computing should not be viewed as a replacement for classical materials modelling. Instead, its most realistic near-term role is as a specialized tool used selectively within larger workflows. The strongest opportunities are likely to emerge where calculating a material's electronic structure creates a bottleneck – as in strongly correlated systems, catalytic reactions and complex interfaces. In this sense, the future is not quantum versus classical computing, but quantum and classical computing operating together.

The background is a dark blue to black gradient, filled with numerous bright blue lines and streaks that radiate from a central point at the bottom, creating a sense of depth and movement. These lines vary in thickness and brightness, some appearing as sharp, straight rays while others are more diffuse and wispy. The overall effect is reminiscent of a high-speed data visualization or a cosmic explosion.

Transdisciplinary
collaboration

Building the infrastructure

Effectively bridging the technologies involved in materials discovery will require new models of collaboration that transcend traditional boundaries between disciplines, institutions, and computational approaches. These collaborative frameworks will be essential for addressing the increasing complexity of materials challenges and leveraging the growing number of computational tools available to researchers.

We propose moving beyond merely “interdisciplinary” approaches, toward truly “transdisciplinary” frameworks where the boundaries between fields become meaningless. This shift requires not just bringing together researchers from different backgrounds but developing shared strategies that enable deeper integration of diverse perspectives.

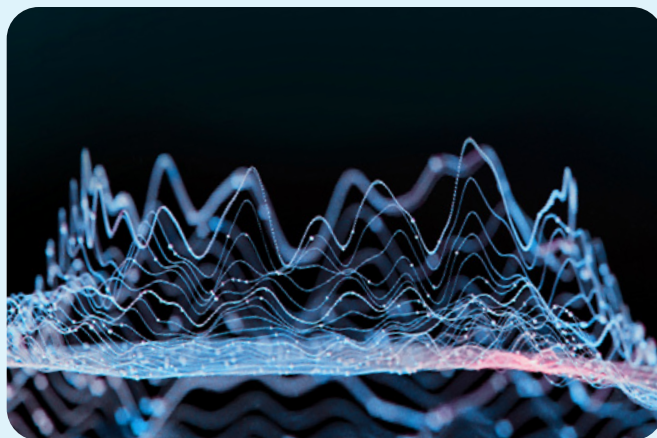
What might transdisciplinary collaboration look like?

Something to consider: What if we organized materials research around properties and applications rather than traditional disciplinary boundaries or computational methods? Such an approach would naturally bring together experts in theory, computation, characterization, and synthesis around specific challenges- creating communities of practice focused on outcomes rather than methodologies.

In this collaborative future, data sharing and interoperability will be critical enablers. Despite progress in materials databases, significant challenges remain in integrating heterogeneous data types, ensuring reproducibility, and creating standards that allow seamless exchange of information between computational tools and across research groups. Technical solutions can help, but the key here will be cultural shifts in how the materials community approaches data sharing.

We envision “computational observatories,” shared platforms that continuously monitor, analyze, and integrate materials data across multiple research groups, creating a dynamic map of the materials landscape. These computational observatories would combine data and results from across the fields of computational studies to create a comprehensive, living resource that supports the discovery process for researchers across disciplines.

The rate-limiting step in materials innovation is increasingly not discovery but knowledge transfer. Our priority for today, then, should be developing more effective collaborative frameworks. This is how we build a materials innovation ecosystem that is greater than the sum of its parts.



A roadmap for coordinated action

The transformative potential of computational approaches in materials science will only be realized through coordinated action across the research ecosystem. Academia, industry, and national laboratories each have their role to play in this transformation.

Academia

For academic institutions, the imperative begins with educational reform – integrating computational methods throughout materials science curricula and developing new degree programs that bridge traditional boundaries.

Quick wins

1. **Revise curricula:** Integrate computational methods across all materials science courses rather than treating them as specialized electives. Ensure every materials scientist graduates with basic computational literacy, as well as experience applying these tools to real materials problems.
2. **Establish cross-disciplinary research clusters:** Create formal structures that bring together materials scientists, computer scientists, and domain experts around specific materials challenges. They can include shared funding, co-supervised students, and joint publication targets.
3. **Develop open benchmark datasets:** Create and publish standardized materials datasets that enable fair comparison of computational methods and algorithms, particularly for emerging approaches like machine learning and quantum computing.
4. **Implement reproducibility standards:** Adopt minimum standards for computational reproducibility in publications, including code availability, environment specifications, and complete parameter documentation.

Transformative change

1. **Pioneer Computational Materials Scientist degree programs:** Develop specialized graduate programs that deeply integrate materials science, computer science, data science, and domain expertise. The goal is creating a new type of researcher specifically trained at this intersection.
2. **Establish materials informatics centers:** Create dedicated research centers focused on developing next-generation computational frameworks that seamlessly integrate across different simulation scales and methodologies.
3. **Redesign tenure and promotion criteria:** Evolve academic incentive structures to reward collaborative, computationally-focused research.
4. **Lead international standardization efforts:** Spearhead the development of international standards for materials data exchange, computational workflows, and benchmarking methodologies that enable more effective collaboration across institutions.

Industry

Industry partners should implement computational approaches from the earliest stages of materials development. This requires not just new tools, but fundamentally rethinking materials innovation processes.

Quick wins

1. **Conduct computational readiness assessments:** Evaluate current R&D workflows to identify opportunities where computational methods could reduce development time and costs, with specific ROI targets for implementation.
2. **Establish academic partnership programs:** Create structured collaboration frameworks with university computational groups, including shared PhD students, visiting scientist positions, and targeted research projects addressing specific industrial challenges.
3. **Develop internal training programs:** Upskill existing materials scientists and engineers in computational methods through dedicated training programs, potentially in partnership with academic institutions or specialized training providers.
4. **Contribute to open materials databases:** Share non-sensitive historical materials data with public repositories. This enhances the training datasets available for machine learning approaches, and also builds goodwill in the research community.

Transformative change

1. **Restructure R&D workflows:** Fundamentally redesign materials development pipelines to integrate computational screening and optimization from the earliest stages, with experimental validation strategically deployed where it adds most value.
2. **Invest in specialized computational infrastructure:** Develop in-house capabilities or secure priority access to advanced computing resources specifically optimized for materials simulations and data analysis.
3. **Create pre-competitive consortia:** Establish industry-wide collaborations on fundamental computational methods and tools that benefit all participants while allowing competition on specific applications and products.
4. **Develop computational digital twins:** Build digital models of manufacturing processes that enable virtual optimization of new materials, accelerating scale-up and reducing costs.

National laboratories

National laboratories are uniquely positioned to develop the next generation of computational infrastructure and integrated user facilities that enable breakthrough discoveries. By creating specialized centers of excellence, training programs, and benchmark challenges, these institutions can accelerate the adoption of advanced computational approaches across the broader materials community.

Quick wins

1. **Launch integrated user programs:** Create user facility programs specifically designed for combined computational-experimental workflows, with coordinated access to both computational resources and characterization facilities.
2. **Establish materials computational Centers of Excellence:** Develop specialized teams and resources focused on helping the broader community apply advanced computational methods to materials challenges.
3. **Create training workshops and bootcamps:** Develop intensive training programs that bring researchers up to speed on state-of-the-art computational approaches, with specific tracks for different experience levels and application areas.
4. **Develop benchmark challenge problems:** Identify specific materials challenges that can serve as standardized test cases for comparing different computational approaches, with associated experimental validation datasets.

Transformative change

1. **Build next-generation computational facilities:** Develop specialized computing infrastructure optimized for materials simulations across scales, including quantum-classical hybrid systems and AI-optimized architectures.
2. **Create national materials digital infrastructure:** Establish comprehensive, interlinked databases and computational platforms that connect materials data across institutions, enabling more effective knowledge sharing and discovery.
3. **Launch moonshot computational materials initiatives:** Identify grand challenge problems (e.g., room-temperature superconductors, revolutionary battery chemistries) where coordinated computational campaigns could drive breakthrough discoveries.
4. **Develop automated materials discovery platforms:** Build integrated systems that combine AI-driven experimental design, robotic synthesis and characterization, and computational analysis in closed-loop discovery systems accessible to the broader research community.



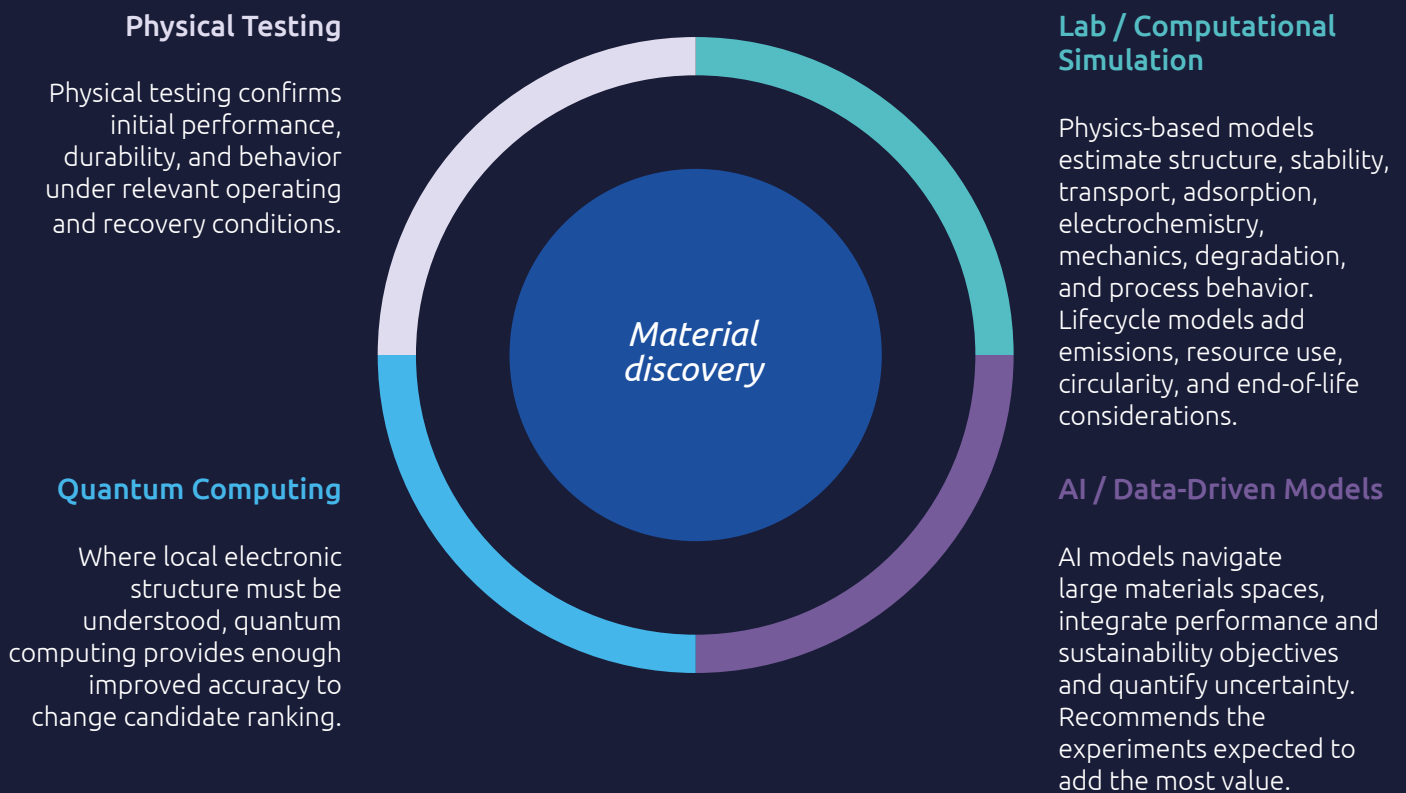
Cross-sector initiatives

Finally, some of the most important initiatives are too broad for any single field to implement on their own. These will require shared effort across sectors.

- 1. Establish a national materials informatics network:** Create a coordinated network connecting academia, industry, and national labs around computational materials science, with shared resources, regular meetings, and collaborative projects.
- 2. Develop common standards and interfaces:** Collaboratively create standards for data formats, computational workflows, and APIs that enable seamless information exchange across institutions and computational platforms.
- 3. Launch joint education initiatives:** Develop educational programs and resources that prepare the next generation of materials scientists for a computational future, with contributions and participation from all sectors.
- 4. Create materials computational challenge prizes:** Establish high-profile competitions with substantial prizes for solving specific computational materials challenges, driving innovation and raising awareness of the field's importance.

In practice: discovering new materials for net-zero energy systems

We typically picture sustainable energy on the scale of infrastructure: windmills, batteries, etc. But each of these systems depends on materials. Metal-organic frameworks for carbon capture provide a prime example: subtle interactions at a local binding site can determine system-level performance. The challenge: candidate materials must combine performance, durability, manufacturability, availability and cost.



Together, AI and simulation explore possible candidates, while sustainability models test their viability. Uncertainty analysis identifies where accuracy matters most, allowing more advanced classical or quantum methods to focus on the most promising options. Physical testing then validates the final shortlist and feeds new data back into the next cycle of discovery.

The evidence base

Illustrative evidence pool: Montgomery, T.W.A. et al. (2025). Accelerating MOF Discovery for Climate Change Mitigation: A Hierarchical Quantum Embedding Approach, developed with TotalEnergies. arXiv:2505.04527. The MOF study illustrates selectively high-accuracy modelling for carbon capture, while the broader vignette concerns a reusable materials-discovery stack supporting energy, utilities, and sustainability outcomes.

See also the companion [multiscale-modelling case study](#) (Section 6, this PoV's parent paper) for the underlying active-space and resource-estimation detail.

Final thoughts

The computational transformation of materials science represents not just an acceleration of discovery but a fundamental shift in how we conceptualize, explore, and ultimately understand materials. This transformation spans multiple dimensions – from the integration of diverse computational approaches to new collaborative frameworks that transcend traditional boundaries.

We believe materials science is approaching an inflection point where computational methods will not just complement but fundamentally reshape the discovery process. This shift will lead us to ask different questions and explore materials space in ways that have never been possible before. The ability to systematically navigate vast compositional landscapes, predict properties across multiple scales, and design materials with specific functional characteristics represents a qualitative change in how materials innovation proceeds.

However, this transformation brings new challenges that the field must address. As computational methods become more sophisticated, ensuring

transparency, reproducibility, and accessibility becomes increasingly important. The risk of creating a divide between computational specialists and the broader materials community is real and could limit the impact of these powerful approaches if not thoughtfully managed.

The central goal isn't faster materials discovery for its own sake, but a deeper understanding of the relationships between structure and function across all materials. Computational methods are most valuable when they go beyond predicting properties, and reveal the underlying principles that govern material behavior – principles that can guide the design of entire classes of materials rather than just individual compositions.

The next breakthrough in materials discovery is unlikely to come from a single technology. It will come from connecting existing capabilities more effectively. AI, simulation, experimentation and quantum computing are individually powerful. Their convergence creates an unprecedented engine for discovery. The future belongs to the organizations that adjust their workflows accordingly.

Contact

Capgemini's Quantum Lab is the company's dedicated team and platform for quantum technology innovation. It offers expertise in quantum computing, quantum chemistry simulations, and post-quantum cryptography. The lab focuses on applying quantum breakthroughs to real business challenges – for example, optimizing complex supply chains or developing quantum-safe security solutions – all with an application-driven approach that ensures practical, sustainable results.

Contact us, and let's discuss how quantum technologies can give your organization the edge.



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About Capgemini

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