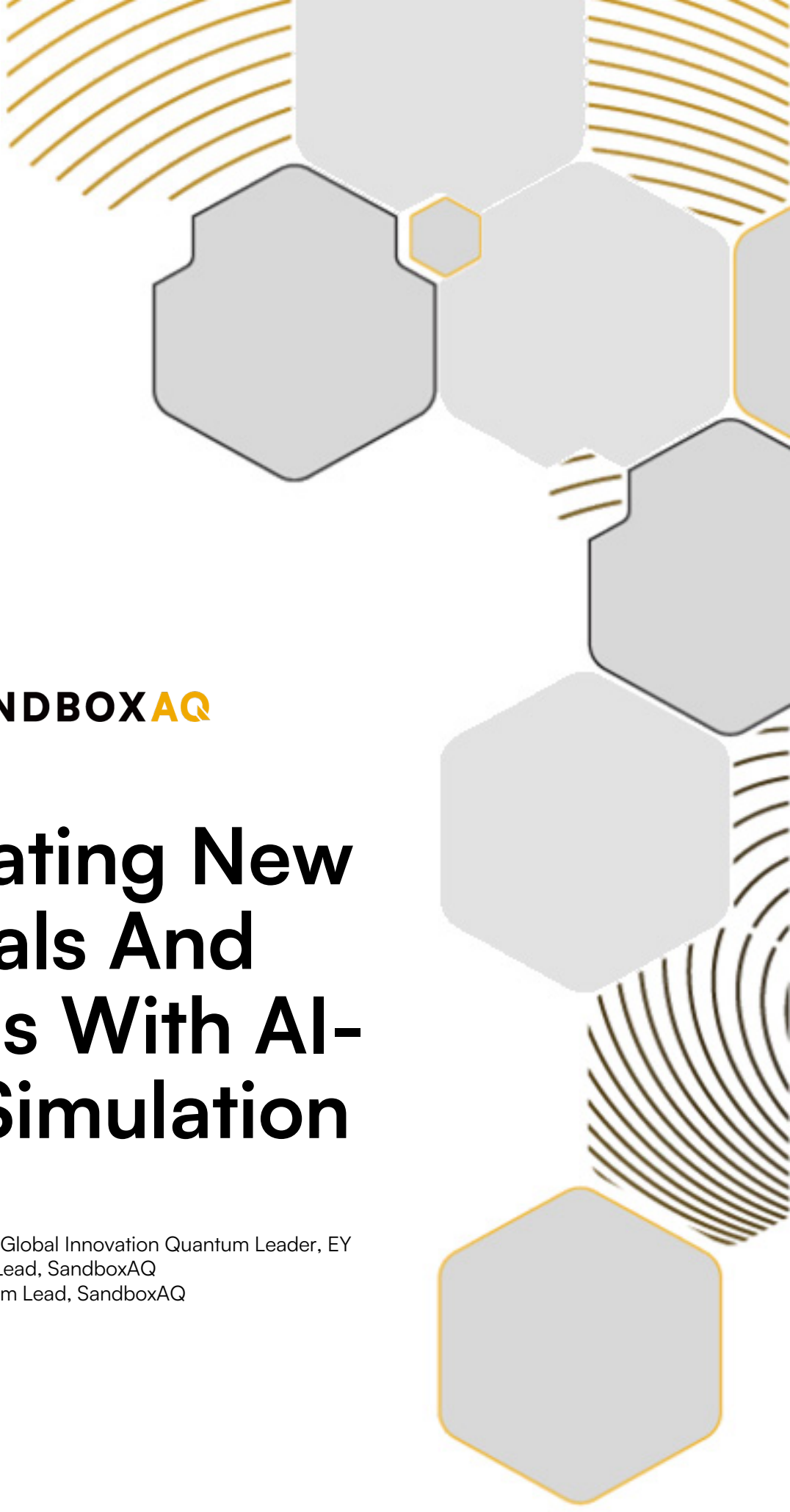

Accelerating New Chemicals And Materials With AI-Driven Simulation

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Executive Summary

Advancements in high-performance computing, AI, and simulation are transforming materials discovery, an industry historically dominated by long and expensive development cycles due to high R&D costs, extensive capital investment in manufacturing, and other barriers.

This paradigm shift, which includes deep learning, graph networks, GPUs, and quantum mechanics simulation techniques, is cutting years off the material science development cycle and significantly reducing costs to bring these breakthroughs to market.

SandboxAQ's AI ChemSim solution integrates AI and simulation, providing a wide range of companies with the tools to conduct in-house materials discovery, drastically reducing cost and time. ChemSim enables users to generate new datasets to train deep learning models, mapping the astronomical chemical spaces, including substances that have never been synthesized or tested before. These datasets are generated by simulating the fundamental dynamics of that type of materials down to the subatomic level.

ChemSim supports a variety of verticals, including catalysts, new alloys and composites for automotive chassis, innovative battery chemistries for both EVs and stationary energy storage, breakthrough materials for clean energy applications such as solar panels, novel materials for building construction, and many others.

This platform enables companies of all sizes to identify new, high-performing materials optimized for product performance, manufacturability at-scale, cost efficiency, and environmental sustainability.

Accelerating Innovation

By harnessing AI's predictive capabilities and extensive datasets, alongside physics-based simulation, enterprises are now able to fast-track the development of innovative materials, positioning them at the leading edge of sustainability and product development.

The chemical and materials industries stand on the brink of a revolution, one where high-performance computing, artificial intelligence, and simulation could power a new era of chemical and materials innovation. [1]

Historically, a handful of conglomerates and academic laboratories have dominated this industry. These giants were the only entities with the resources to carry out costly, time-consuming R&D and scale up manufacturing processes, with no guarantee of success. In addition, development teams lacked computations tools to model new material
at scale and with sufficient dynamics. As a consequence, innovation has been sluggish.

Innovation is now accelerating with the advent of high-powered computing (HPC) and AI which are democratizing and supercharging chemistry and materials science. Armed with deep learning techniques, graph network models, GPUs, and novel large-scale Density Functional Theory (DFT) and Molecular Dynamics (MD), companies of all sizes can afford to compete and innovate. [2, 3] Whatever complex factors they are optimizing for, AI and simulation methods can help you do it faster, more affordably, and at scale.

Using AI with extensive testing and verification, a tool could mean irrespective of size, can predict new material compositions at scale. And by extension, a certain number of them are potentially useful in improving product performance, cost efficiency, and raw material scarcity. Even identifying alternative materials that are either healthier or cleaner for the planet.

While the technology still requires scientist oversight and quality assurance [9], the ability for deep and machine learning models to predict and test new materials faster and at scale means broad democratization of materials discovery.

What is Simulation?

AI-driven simulation in materials science involves leveraging artificial intelligence to enhance the accuracy and efficiency of identifying new materials through understanding their complex molecular behavior. Historically, material science experiments and simulations can be time-consuming and costly. The emergence of the AI-driven counterpart streamlines this process by employing machine learning models, deep learning techniques, graph network models, and more to predict material behaviors, properties, and interactions.

Using machine and deep learning, researchers can prognosticate material behaviors by identifying patterns and relationships within large datasets covering material properties, structures, and performance metrics. These simulation models use algorithms that recognize complex patterns and make predictions based on the input data, thus suggesting new materials or variants of existing ones.

With AI-driven simulation researchers can virtually test—in silico as opposed to lab-based in vitro testing—and discover greater details about the matter, materials, and their interactions, down to the quantum mechanical level.

Running on distributed networks and featuring the latest generation of classical GPUs, enterprise SaaS company SandboxAQ merges quantum-inspired solutions and quantum chemistry toolkits with AI computation, democratizing materials discovery through physics-informed simulation and machine learning. Effectively enabling any manufacturing company to move the expensive and time-intensive materials discovery process in-house.

SandboxAQ's solutions employ a range of techniques including tensor networks, quantum chemistry toolkits, generative modeling, and natural language processing to offer companies and R&D labs the tools to deliver groundbreaking, accelerated results in materials science and product development.

What Is AI-Powered Materials Discovery?

Chemical and materials science is about the development and characterization of new substances for use and industry consumption—everything from metals, alloys, ceramics, and polymers to fuels, batteries, and composites.

Three Examples of Innovations in Materials Science and Their Impact:

1. The invention of nylon, initially for the production of parachutes, created an entire market segment of polymer materials.
2. Semiconductor innovations are at the heart of the computer chip industry.
3. Future materials such as room-temperature superconductors could usher in a new technological era for sectors including energy transmission and storage, helping us combat climate change.

Innovations and discoveries in the chemicals and materials space can create significant new value without the requirement of being a multinational corporation.

However, in large part, serendipity has driven materials change and innovation, where unexpected discoveries or observations have led to groundbreaking advancements.

Notable cases of this serendipity include the discovery of Teflon in the 1930s by chemist Roy Plunkett, who was working on refrigerants at the time, and the discovery of Gore-Tex in 1969 by engineer Robert Gore, who stumbled upon expanded polytetrafluoroethylene (PTFE) as a waterproof fabric.

Systemic research and deliberate experimentation are pushing innovation in chemicals and materials science, and in this capacity, gate-kept by large corporations, possessing the edge of resources, patents, and capital to dominate traditional materials research and discovery.

Thus, the need for widening materials innovation availability is vitally important for enterprises of all sizes. The search for new materials is ramping up in response to demand from areas such as technology, where shortages of sought-after materials and rare earth metals are becoming scarcer. Manufacturers also have to contend with continuously changing government regulations, where jurisdictions call for new substitute materials in the face of scarcity, health damage, and/or environmental concerns. [4]

Fortunately, advances in AI and simulation hold significant promise to usher in a new democratized era of materials discovery [5]—one that is far more accessible to companies without the resources of large multinationals.

Physics-based simulation uses computational methods based on the principles of physics to model and simulate the behavior of materials, molecules, and chemical processes. The aim is to predict dynamics at the atomic and molecular levels to gain insights into the properties of materials and chemicals without the need for extensive experimental testing.

A main advantage of physics-based simulation is that it requires relatively small pools of training data to provide accurate results, and as computing power increases over time, this approach proves more valuable for materials discovery. But although it has been used for decades, the practice has been more or less restricted to specialized researchers in R&D-heavy industries, as the necessary computational power is large and costly and the research requires specialized hardware.

AI-enabled simulation promises to mitigate these costs and challenges, representing a paradigm shift in materials discovery. AI simulation is data-driven, leveraging machine learning models trained on diverse datasets—and doing so at incredible speed and less cost. High-throughput screening and the exploration of a vast parameter space are keys to this approach to optimizing new materials discovery.

AI SIMULATION

PROS: less time-consuming than physics-based modeling; highly versatile and efficient in data integration and identifying novel material compositions

CONS: low accuracy compared to physics-based methods; bias-prone dependency on the quality and representativeness of training data. Yet, this can be accounted for in its usage.

As access to data and compute power grow, AI simulation methods are improving in tandem, driven by the rise in the use of GPUs and deep learning models. AI systems such as Large Language Models are helping to circumvent the need for specific, predicted experiment data. For example, synthetic data approaches employ physics-based methods to produce training data sets for consumption by AI models, whereas physics-informed neural networks use physics-based models to filter outputs to conform to the laws of physics.

SandboxAQ operates at the intersection between physics-based simulation and artificial intelligence, identifying continued synergies and compound effects between the two emerging technologies. Our simulation and optimization platform combines the strengths of physics-based simulation and AI-driven modeling to provide companies the capabilities to move materials discovery in-house, opening up new opportunities for vertical integration and with it, numerous benefits.

SandboxAQ is collaborating with GPU-maker NVIDIA on simulating quantum mechanics for use in molecular and materials research. Announced in November 2023, the collaboration will see SandboxAQ providing technical recommendations on NVIDIA tensor networks and algorithms, running highly GPU-optimized tensor network methods on NVIDIA GPUs to represent high-dimensional data with potential applications in the creation of new materials and chemical compounds.

This enables SandboxAQ, with the backing of NVIDIA, to provide strategic business value to general manufacturers in materials discovery by preventing manufacturing companies from outsourcing their materials discovery and product innovation.

How Simulation and AI Impact Materials Discovery

What are the Problems With Material Discovery?

Despite incredible progress, researchers in chemical and materials discovery face significant challenges that impede the pace of its development.[6]

THE MATERIALS INFORMATICS PROBLEM

One difficulty involves the complexity of predicting material properties and behaviors at the atomic level. Quantum mechanics provides a theoretical framework for understanding these properties, but the computational power required to model complex systems accurately is, for now, untenable.

This bottleneck is known as the materials informatics problem, where handling the multidimensional spaces of chemical compositions, structures and processing conditions is computationally intensive and requires sophisticated algorithms. Moreover, the synthesis of new materials often involves trial and error and requires exploration of a vast array of potential combinations and reactions, further exacerbating the complexity.

BETTER TOOLS FOR HIGH-THROUGHPUT SCREENING

The need for better high-throughput screening (HTS) methods presents another challenge. Used in areas such as drug discovery and materials research, HTS has traditionally involved physical lab work with large numbers of chemical compounds or biological agents, where researchers test these compounds for a targeted biological or chemical activity. Over the years, HTS has become more linked with in silico computational setups, where computer modeling takes the place of actual lab work.

But HTS faces hurdles, since the computational power needed to accurately simulate physical systems is large, and programs often lack high-quality, diverse data upon which to base the models. These issues can affect the accuracy and predictability of HTS.

LIMITATIONS AND COSTS OF MODELING

Another challenge stems from the intrinsic limitation of characterization techniques. To understand new materials at a granular level, researchers need specialized tools that can probe the atomic scale, such as advanced electron microscopy or synchrotron-based spectroscopy. However, this type of equipment is not only expensive and limited in availability, but it also might not provide sufficient resolution or contrast for all materials of interest These spectroscopic techniques also require specific sample preparation and conditions, which may not always be achievable for the materials being studied.

Moreover, expense can limit the number of players in the field, and even when smaller companies do pursue materials discovery, it is often conducted in partnership with a larger chemical and materials R&D company, which in turn regularly requires that the smaller business cede at least partial research control and IP to the larger entity.

INTERDISCIPLINARITY AND SUSTAINABILITY

The interdisciplinary nature of modern materials science can pose a cultural and organizational challenge. Effective communication and collaboration across chemistry, physics, engineering, and computational science are critical to the work yet can be hindered by differing terminologies, methodologies, and objectives. Additionally, the training required for researchers to span these diverse fields is extensive, creating a scarcity of individuals who can bridge the gaps and drive the necessary collaborative breakthroughs.

In recent years, environmentally responsible synthesis pathways, lifecycle assessments, and recyclability of materials have become mandatory considerations for chemical and materials research. Yet, the integration of sustainability into the discovery process is an issue and often requires the development of entirely new synthesis methods that are both green and economically feasible.[7]

Simulation and AI in Materials Discovery

AI techniques and high-power computing chemistry methods are particularly useful in addressing these challenges to materials discovery. As AI simulation and chemistry advances, these could become valuable in the future.

MATERIALS INFORMATICS

AI and machine learning can identify patterns and predict material properties quicker than traditional methods which are limited to high-quality data to interpolate and extrapolate to a broader chemical space. AI thus reduces dependency on exhaustive empirical testing. Meanwhile, quantum mechanics simulation could lead to more accurate predictions of material behaviors and properties.[5]

HIGH-THROUGHPUT SCREENING

AI and DFT-based quantum mechanics simulation are particularly adept at enhancing HTS. They enable automated analyses of large datasets generated by combinatorial chemistry and high-throughput experiments, identifying promising candidates at an accelerated pace. When integrated with robotics and automated laboratory systems, these techniques can lead to a significant increase in the speed of experimental material synthesis and characterization.[7]

LIMITATIONS AND COSTS OF MODELING

Advanced data processing algorithms can extract meaningful insights from noisy or incomplete data. AI can also help in the design of experiments to maximize the information gained from these high-end tools, optimizing the use of available resources.[7]

INTERDISCIPLINARITY AND SUSTAINABILITY

AI can process and analyze data from different scientific domains, providing a common ground for different experts to collaborate effectively. Researchers can use cloud-based platforms and collaborative software to seamlessly share computational resources and data, bringing together chemists, physicists, materials scientists, and engineers to work on shared objectives. Researchers can address sustainability concerns by leveraging AI and machine learning to assess and optimize the environmental impact of new materials throughout their lifecycle.[8]

What is Quantum Technology?

Quantum technologies use the perplexing properties of matter at the quantum level—such as superposition, entanglement and quantum coherence—to deliver fascinating and potentially practical results in computation.

Highly precise quantum-based sensors, for example, are used in fields like space science, medical imaging, meteorology, and environmental monitoring. And quantum computing, while still in the early stages of its maturation, may provide accelerated processing and a new paradigm of computing, using information units called qubits (quantum bits) rather than the traditional digital bits (ones and zeros) used in classical computing.

Simulation on high-performance classical computing systems that use quantum mechanical principles can mimic the behavior of quantum systems. Quantum algorithms implemented on quantum computers, can be a powerful tool in fields like generative chemistry, where researchers strive to discover new chemical structures and protein binding affinities.

The Benefits of Simulation and AI on Materials Discovery

By deploying AI, quantum-inspired solutions and quantum chemistry toolkits strategically, companies can lower many of the barriers to progress in chemicals and materials discovery. These technologies not only accelerate the pace of discovery and the time-to-value but also promote efficiency and sustainability.

Physics-based simulation and AI can lead to new and improved material discovery while widening accessibility and empowering companies toward scientific advancement and product development.

BENEFITS OF AI-DRIVEN SIMULATION

1. Moves material discovery in-house, opening possibilities for vertical integration and mitigating risks from using a dedicated partner.
2. Increases the leads' control of their material discovery and alignment with their current and future products.
3. Saves overall costs of material discovery.
4. Improves speed of material discovery and innovation from rapid testing.
5. Enables more elaborate new and existing product development, plus linked market strategies from product-market fit.
6. Enables smaller companies to employ material replacements, for example, from changing material regulations.

SandboxAQ has powerful tools for companies looking to make breakthroughs in material science. Sandbox's AI-driven simulation technology creates virtual libraries of molecules and compounds, and runs millions of simulations to predict physical and chemical properties, while its advanced AI analyzes and optimizes those findings for use in materials discovery.

The approach to AI adopted by EY

Build confidence in AI

Leverage robust frameworks and governance that instill confidence and empower responsible transformation.

Create exponential value

Optimize performance, enrich customer and employee experiences, and unlock new sources of sustainable growth.

Augment people potential

Create a future where seamless people-AI collaboration achieves extraordinary outcomes.

EY Fabric: Powering EY.ai

Our global foundational technology platform embeds EY.ai with leading-edge AI capabilities, united robust data strategies, cloud hyperscalers, and efficient AI management. Its rigorous AI governance ensures responsible and ethical AI use, setting new industry benchmarks.

The range of possible applications is endless, running the gamut from construction and manufacturing to agriculture, transportation and energy. The search for stronger, lighter, aerodynamic, thermodynamic, more durable and environmentally-friendly materials starts with SandboxAQ.

SandboxAQ announced in September 2023 a collaboration with battery materials and technology company NOVONIX, to use SandboxAQ's AI-driven chemical simulation to help develop new technologies and materials for lithium-ion batteries.

Battery performance and degradation are common testing grounds for companies looking to enhance battery quality, but these lifetime and performance assessments in aid of improving chemical and material improvements can be time-consuming. With SandboxAQ's simulation software and NOVONIX's proprietary battery data platform, research groups and companies can get actionable information faster, leading to accelerated product development timelines.

> "Simulation will drive a new wave of GPU use, powering previously unattainable insights about our physical world that go beyond what extractive or generative AI are capable of unlocking. Combining Simulation with advanced AI yields solutions to problems in some of the biggest addressable markets in the world, far beyond what generative AI is capable of doing alone," said Jack D. Hidary, CEO of SandboxAQ.

Case Studies

More efficient and selective organometallic catalyst

Challenge: Finding optimal Ni/Fe Carboxylate organometallic catalyst in a library with millions of ligands for a global chemicals company

Solution: Using our enterprise SaaS platform (SandboxAQ QEMIST[™] Cloud hosted on AWS), we predicted the binding energy of millions of ligands with the transition metal center in silico. We down-selected the optimal candidates in two months instead of multiple years, leading to 90%+ savings in time and experimental costs.

Battery cycle life prediction

Challenge: Predicting battery degradation is pivotal for advancing material research and unlocking opportunities in battery design, testing, and recovery, but traditional approaches often fall short.

Solution: We utilized a Graph Neural Network (GNN), integrating time-series experimental data from thousands of commercial cylindrical and prismatic cells, to accurately predict battery performance degradation.

1 Million+ core PFAS elimination simulation

Challenge: Enabling a Fortune 500 company to reduce their waste PFAS output by 90%+ by modeling Carbon-Fluorine bond dissociation energies that had been unattainable on the cloud

Solution: We applied SandboxAQ's unique iFCI algorithms and 1 million+ CPU cores on AWS to accurately predict the dissociation energy of alpha C-F bond of PFOA (perfluorooctanoic acid). This is one of the most potent and persistent chemicals artificially made in the world. SandboxAQ provides experimental chemists new avenues to reduce 90% of this forever chemical in the environment, saving billions of dollars for environmental cleanup and remediation efforts needed to remove PFAS from contaminated water sources. It also means billions of dollars saved in annual healthcare costs by reducing illnesses linked to PFAS exposure, including cancers and liver damage.

Discovery of new cathodes for SOFC (solid oxide fuel cells)

Challenge: Selecting materials with superior oxygen kinetics from millions of compositions and processing conditions

Solution: We developed a funnel-based searching process over tens of thousands of materials to find promising perovskites. Applying rigorous criteria related to activity, stability, and conductivity, we narrowed down to a set of materials with high potential for oxygen reduction reactions. One of these materials, BFCZ75, displays state-of-the-art cell performance, outperforming many existing materials with significantly higher conductivity and lower resistance.

Conclusion

With the power of emerging technologies in AI-driven simulation, making breakthroughs in the chemicals and materials space is becoming more realizable and more accessible.

Companies and research groups will gain an advantage by incorporating physics-based simulation and AI into their research programs, cutting years and capital off the development cycle. Companies can use this platform to do in-house in a short period what would previously take years of outsourcing. By collaborating with EY and SandboxAQ, you can position yourself at the forefront of innovation.

Contact us today to discover more about how EY and SandboxAQ leverage AI simulation to support businesses in proprietary material discovery and how your general manufacturing processes can benefit from AI-driven materials discovery.

Contact our team.

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