

# A recipe for future success? How Data and AI are changing materials innovation

Picture a delicious bowl of ramen. It's been perfected by a shop owner over many years. The taste comes from experience, daily trial and error, and small adjustments along the way. But the recipe was never written down, and no one can reproduce it exactly. What's more, a slight change in temperature, one of the ingredients, or even how it's stirred creates a "one-time-only" taste that can't be replicated.

This story mirrors a common reality in the world of materials development.

Many breakthroughs come from the skills and intuition of experienced researchers. But when the reasoning behind these successes remains a "black box," repeating or predicting results becomes extremely difficult. For companies to grow sustainably in uncertain times, they need to move beyond relying on individual expertise. Instead, they must uncover and define the real principles — the causal relationships between materials and their functions.

This is where Materials Informatics (MI) comes in. MI isn't just about using new tools. It's a fundamental shift in how materials are developed: moving from trial-and-error "recipe hunting" to principle-based development that's grounded in data and clear logic. This shift makes manufacturing more predictable, more efficient, and more reliable.

MI is built on data infrastructure and artificial intelligence (AI), strengthened by high-performance computing (HPC) and quantum computing, which will play a growing role in future innovation. When these technologies are used together in a coordinated way, their impact is much greater than when used separately.

The benefits of MI go well beyond faster analysis or more accurate testing. MI helps create the foundation for a next-generation manufacturing system — one where experiments can be planned and carried out automatically, and results can be verified through robotics and automation.

Fujitsu is driving this change with advanced AI technologies, including explainable AI, causal discovery AI, and AI agents. We also bring decades of experience in data management and HPC, along with a strong R&D program in quantum technology.

This report explains how MI is transforming materials development, highlights global trends, and introduces the key technologies behind this shift. It also outlines Fujitsu's approach to making MI more effective.

To build the future we want, we need to move from trial and error to principle-based development. Now is the time to take the first step toward a stronger, more sustainable competitive edge. This is the recipe for success.

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## Section 1

# Unlocking the core “Why” in materials development

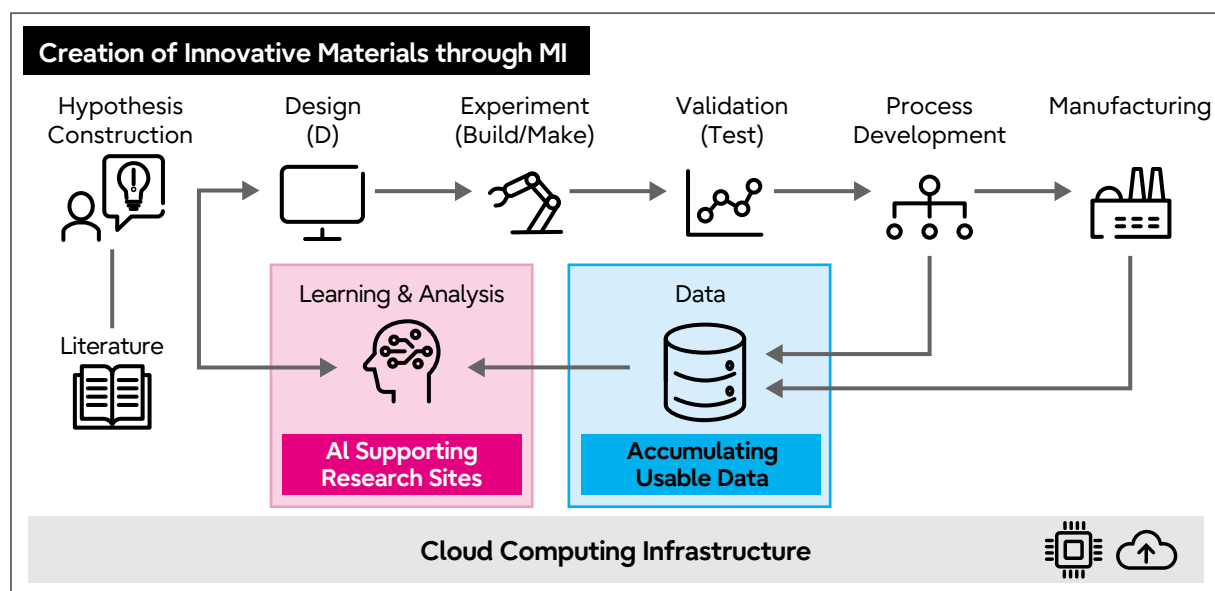
At its core, Materials Informatics (MI) is a strategic and practical approach designed to fundamentally transform the entire lifecycle of materials—from design and development to manufacturing—by leveraging the power of data and advanced technology.

A significant challenge in conventional materials development often stems from a “black box” phenomenon. While specific formulations and processes (the “How-to”) derived from the extensive knowledge and experience of seasoned researchers, or even serendipitous discoveries, undoubtedly represent valuable corporate assets, their true potential is limited if the underlying causal relationships remain opaque. This ambiguity severely restricts reproducibility and forces organizations to address new challenges in a trial-and-error fashion, akin to navigating uncharted waters without guidance.

MI aims to disrupt this traditional “recipe-seeking” paradigm in materials development. Its primary objective is to illuminate the fundamental question: “Why do specific material properties manifest?”—unveiling the core “Why,” or underlying principles (Figure 1).

“Principles” in this context refer to the essential causal relationships, physical and chemical laws, and foundational design rules that govern material properties. Through the application of data, AI, and simulation tools, MI strives to extract universal knowledge previously obscured within the “black box.” The goal is to establish objective laws that define how micro-level structures, such as atoms and molecules, influence macro-level functions and performance. Once these principles are clarified, organizations can design materials with a blueprint-like precision to achieve desired characteristics. This critical shift in mindset, perspective, and action—from merely knowing “How-to” to deeply understanding “Why”—is essential for infusing true intelligence into materials development.

**Figure 1: Revolutionizing the entire materials development process with data, AI, and cloud technologies**



(Source: Fujitsu)

## ■ Expanding applications across diverse industries and fields

The transformative impact of MI is poised to extend across a myriad of industries and sectors (Table 1).

**Table 1: MI: A catalyst for innovation across diverse industrial sectors**

| Main industries       | Main Development Areas                                                                                                                                                               |                                                                                                                                         |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Chemicals & Materials | <ul style="list-style-type: none"><li>• High-performance polymers</li><li>• Coatings, inks, adhesives</li></ul>                                                                      | <ul style="list-style-type: none"><li>• Surfactants, additives</li></ul>                                                                |
| Automotive            | <ul style="list-style-type: none"><li>• Lightweight, high-strength materials</li><li>• High-performance battery materials</li></ul>                                                  | <ul style="list-style-type: none"><li>• Improved durability of fuel cell materials</li></ul>                                            |
| Aerospace             | <ul style="list-style-type: none"><li>• Superalloys and composite materials resistant to extreme environments</li><li>• Structural weight reduction and safety enhancement</li></ul> | <ul style="list-style-type: none"><li>• Corrosion-resistant and wear-resistant materials</li></ul>                                      |
| Medical & Healthcare  | <ul style="list-style-type: none"><li>• Highly biocompatible biomaterials</li></ul>                                                                                                  | <ul style="list-style-type: none"><li>• New sensor materials for diagnostic applications</li></ul>                                      |
| Electronics           | <ul style="list-style-type: none"><li>• Enhanced performance of semiconductor materials</li><li>• Improved functionality of display materials</li></ul>                              | <ul style="list-style-type: none"><li>• Materials for next-generation communication (dielectrics and high-frequency response)</li></ul> |
| Energy                | <ul style="list-style-type: none"><li>• High-efficiency solar cell materials</li><li>• Materials for next-generation energy storage devices</li></ul>                                | <ul style="list-style-type: none"><li>• Nuclear fusion</li><li>• New catalysts for carbon neutrality</li></ul>                          |

(Source: Fujitsu)

While the adoption of MI is steadily growing across various domains, its implementation often remains localized within many organizations and research institutions. This situation, however, presents a significant strategic opportunity for pioneering companies to enhance their market valuation and secure a substantial competitive advantage.

MI-driven transformation promises to considerably reduce both the development cycle time and associated costs for new materials, thereby accelerating the creation of groundbreaking innovations. Furthermore, it will play a crucial role in overcoming resource limitations and mitigating environmental impact. Ultimately, MI possesses the capacity to robustly support both the sustainable growth of enterprises and the realization of a sustainable society, simultaneously.



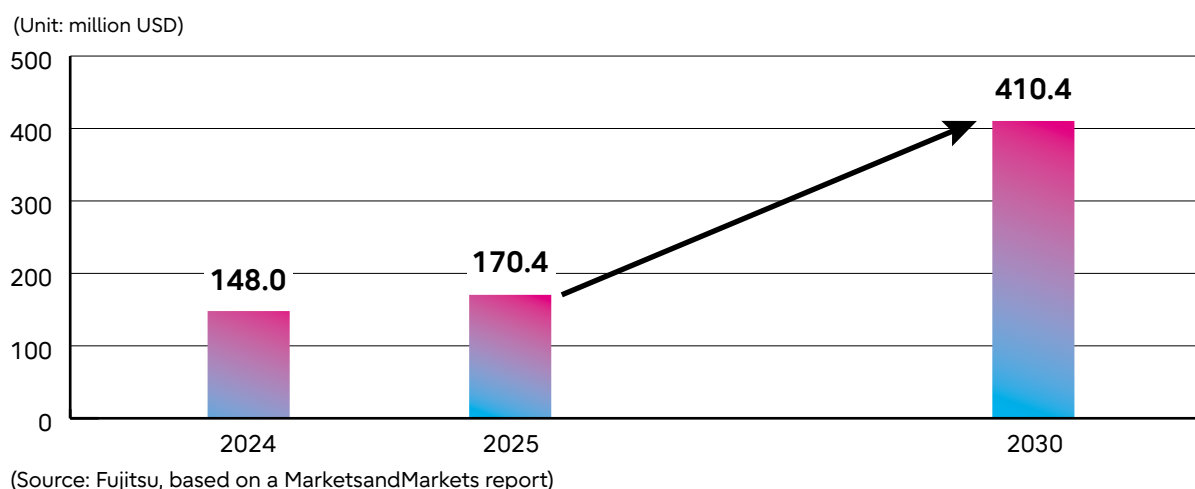
## Section 2

# Expanding markets, expanding AI

The Materials Informatics (MI) market is recognized as one of the most rapidly growing sectors globally.

According to the report “Material Informatics Market Size, Share & Trends, 2025 To 2030\*<sup>1</sup>” published by MarketsandMarkets in 2025, the global MI market size is projected to expand from USD 170.4 million in 2025 to USD 410.4 million by 2030. This growth translates to a notable Compound Annual Growth Rate (CAGR) of 19.2% during the forecast period (Figure 2).

**Figure 2: The MI market is projected to grow at a compound annual growth rate approaching 20%.**



AI is indispensable for the effective implementation of MI. According to a 2025 report by 360iResearch,

“AI in Chemical & Material Informatics Market”<sup>2</sup>, the market size for AI in chemistry and MI is estimated to surge from USD 17.1 billion in 2025 to USD 89.66 billion by 2030. The report highlights that “industry practitioners are witnessing several transformative changes that elevate AI from experimental support to strategic capability.”

## ■ The transformative impact of materials informatics

How does the effective implementation of MI, coupled with the optimal utilization of AI, drive “transformative changes”? Below, we outline the primary impacts that MI delivers:

- **Accelerated development and cost reduction:**  
Significantly shortens time-to-market and reduces investment, providing a substantial competitive advantage.
- **Expanded opportunities for novel material creation:**  
Enables the exploration of “unknown material spaces” that are beyond the reach of human intuition and experience alone.
- **Optimized supply chains:**  
Contributes to improved yield rates through more accurate material property predictions. Furthermore, by establishing highly efficient resource recovery processes from used fuels and materials, it supports the realization of a circular economy.



- **Evolution of ecosystems and R&D frameworks:**

Positions MI as a foundational element for societal transformation, fostering industry-academia collaboration between companies, universities, and research institutions. This facilitates the establishment of frameworks to swiftly integrate new insights and technologies into practical application.

The benefits of these impacts are severely limited if technological adoption is confined to isolated areas. Moreover, in an era characterized by intricately linked business challenges, achieving MI transformation in isolation as a single company is exceptionally difficult. Success hinges on enabling synergistic collaboration across various technologies and partnering with like-minded companies and organizations. A flexible and agile approach to thinking and execution will enhance MI's practical efficacy and ensure a sustained competitive advantage.

\*1 Material Informatics Market Size, Share & Trends, 2025 To 2030

<https://www.marketsandmarkets.com/Market-Reports/material-informatics-market-237816259.html>

\*2 AI in Chemical & Material Informatics Market

<https://www.360iresearch.com/library/intelligence/ai-in-chemical-material-informatics>



## Section 3

# Technologies accelerating materials informatics transformation

The transformation driven by Materials Informatics (MI) significantly enhances its practical efficacy by optimally leveraging and interconnecting multiple technologies. Data infrastructure, AI technology, High-Performance Computing (HPC) including supercomputers, and quantum computers are positioned as the central pillars fostering a virtuous cycle of MI transformation. Accelerating the shift from “recipe-seeking” to “principle-driven” approaches through these technologies is what truly brings intelligence to materials development.

### ■ Data infrastructure: A strategic reservoir of knowledge for unveiling principles

Data serves as a “strategic reservoir of knowledge” critical for unraveling the principles of materials development, and it is a decisive factor in determining AI's performance. A robust data infrastructure is therefore indispensable as the fundamental bedrock of MI transformation.

- **Quality and quantity:** For MI to function effectively, both the abundance of data and, critically, its high quality are paramount. Merely accumulating unreliable data will only lead to flawed insights. It is essential to integrate diverse experimental and simulation results through data standardization and reliability assessment to derive valuable inherent principles.
- **Database construction:** Structuring and centrally managing disparate research, measurement, and simulation data within a unified database is crucial. The effective utilization of public databases, alongside securely accumulating and sharing proprietary data via private databases, actively promotes the systematization of knowledge.
- **Data preprocessing technology:** Preprocessing techniques such as imputation for missing values, noise removal, and normalization—all essential for transforming data into an AI-ready format—are pivotal in determining AI's learning efficiency and prediction accuracy. The presence of high-quality data preprocessing technology fundamentally dictates the depth of principles derivable through MI.

### ■ AI technology: Driving knowledge discovery by uncovering laws hidden in data

AI technology forms the core of MI. It assumes the role of a “knowledge explorer,” actively seeking out and deriving principles that lie hidden beneath conventional recipes. AI clarifies subtle patterns and complex causal relationships embedded within data that are often imperceptible to humans, thereby providing concrete and clear explanations and insights for material design.

- **Advanced AI models:** Graph Neural Networks (GNNs) are highly effective in representing atomic and molecular structures, thus improving the accuracy of material property predictions. Bayesian optimization and transfer learning support efficient optimal material exploration even with limited datasets. Reinforcement learning significantly increases the potential for AI to identify optimal development procedures and manufacturing methods for materials with desired characteristics through iterative trial and error.
- **Explainable AI (XAI):** Even highly accurate AI predictions are challenging to utilize if their underlying reasoning is unclear. XAI provides the capability to visualize and present AI's prediction logic in a human-understandable format. This enables AI proposals to be leveraged not merely as “results” but as crucial “hints” for forming new hypotheses and discovering fundamental principles.
- **Causal discovery AI:** To genuinely uncover principles, it is imperative to identify true causal relationships, not just mere correlations. Causal discovery AI opens new avenues by statistically estimating causal relationships from data, thereby revealing fundamental mechanisms behind

phenomena previously understood only empirically. It plays a critical role in elevating material design from reliance on empirical rules to achieving genuine scientific foundations.

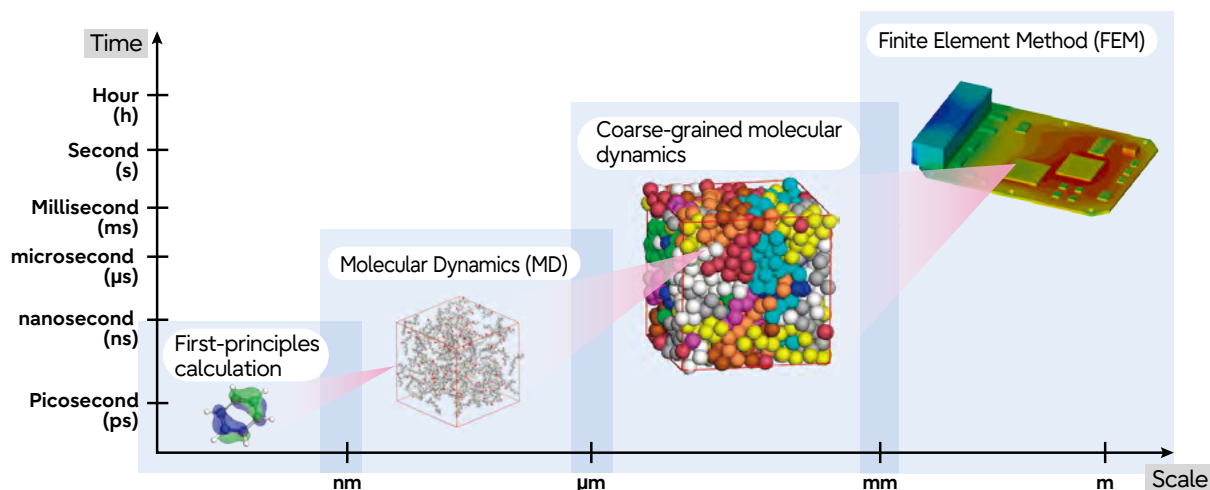
- **AI Agents:** AI agents hold the potential to autonomously drive the entire materials development cycle. This encompasses AI independently generating hypotheses, formulating optimal experimental plans, controlling robotic experimental systems, conducting experiments, learning from results, and then optimizing conditions for subsequent experiments—an autonomous, iterative process. Autonomous AI-driven experimentation not only shortens development times and reduces costs but also addresses labor shortages, boosts productivity, and optimizes processes, thereby constituting a vital component of the “next-generation manufacturing operation system.”

### ■ HPC: Supercomputer simulations as a key enabler for MI transformation

While AI excels at discovering principles from data, simulations powered by HPC serve as a potent engine for MI transformation, verifying existing principles and enabling further predictions. The physical and chemical behaviors of materials are extraordinarily complex. HPC replicates and predicts behaviors in a virtual environment—such as extreme conditions and microscopic phenomena—that are beyond the scope of conventional experimentation. By accurately evaluating the properties of AI-proposed material candidates and generating synthetic data for AI model training, HPC facilitates an ultra-fast MI cycle.

- **Large-scale computing capability:** HPC executes calculations across all scales at high speed, from complex quantum chemical computations and molecular dynamics (MD) simulations tracking millions of atoms, to continuum analysis predicting product-level responses. Its immense computing power broadens material design possibilities, allowing for the efficient exploration of specific pathways towards a “desired future”—ideas that would be unattainable through human effort alone—all within a virtual world.
- **Multiscale simulation:** Material functions manifest across a spectrum of spatial and temporal scales, ranging from atomic and molecular behavior to crystal structures, microstructures, and the macroscopic properties of final products. HPC enables “multiscale simulation” by integrating and linking computational methods tailored to each scale, such as first-principles calculations (electronic states and behavior), molecular dynamics (atomic and molecular motion), coarse-grained molecular dynamics (behavior and self-organization of atomic and molecular assemblies), and finite element methods (deformation of entire structures). This approach consistently predicts material properties from the atomic to the product level based on unified physical laws, leading to a profound understanding of underlying principles (Figure 3).

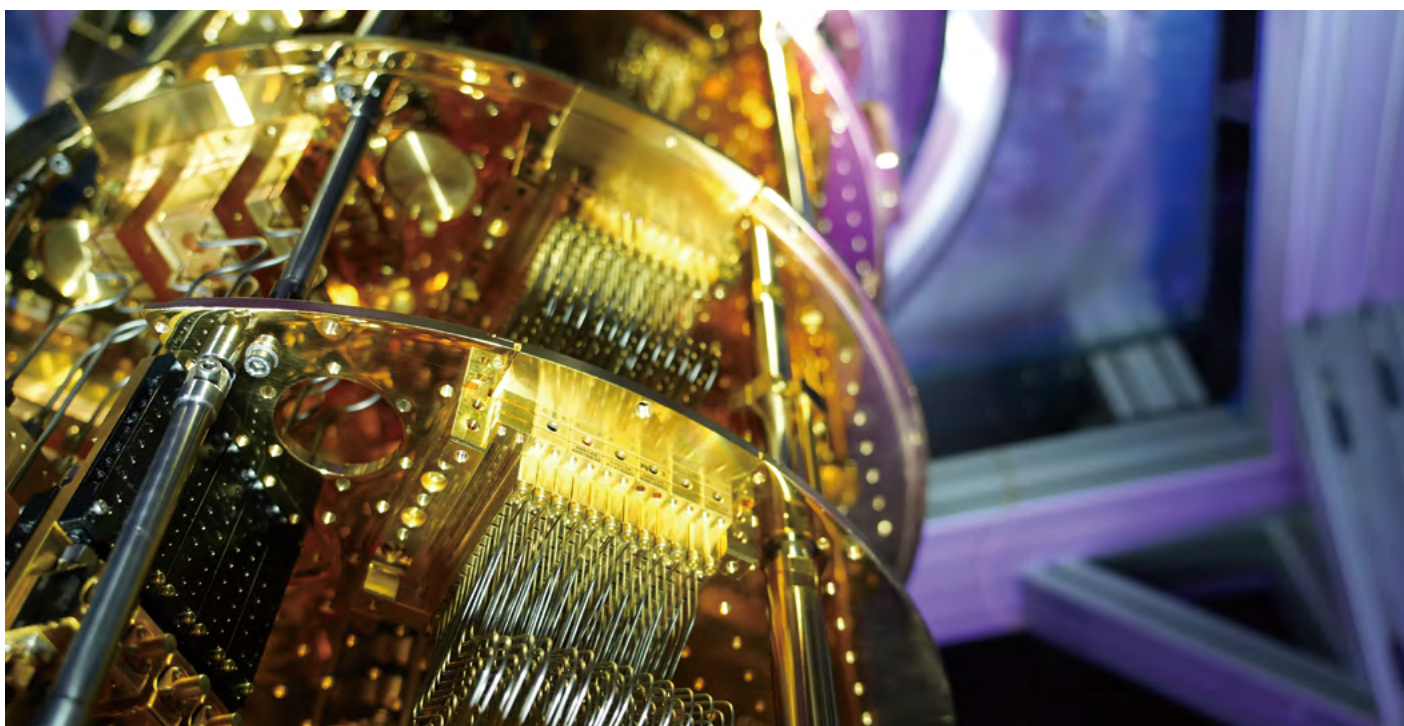
**Figure 3: Multiscale simulation integrating computational methods across different scales**





## ■ Quantum computers: The next-generation engine for MI, beyond current performance limits

Quantum computers possess the potential to redefine future materials science by breaking through computational barriers that existing technologies cannot overcome. Although quantum computers are still in the developmental stage, they are not a distant future technology. As a next-generation engine for MI transformation in the near future, they are poised to bring breakthroughs to the world of material design. Engaging in research and development of quantum technology now and actively pursuing use case development with quantum applications designed for actual corporate deployment, will significantly enhance competitive advantage.



## Section 4

# Fujitsu's integrated approach to implementing materials informatics

Materials Informatics (MI) transformation necessitates the optimal combination of data infrastructure, AI technology, HPC simulations, and, in the near future, quantum computing. This chapter details how Fujitsu intends to leverage these accumulated technologies and practical expertise to drive MI transformation effectively through its unique approach.

### ■ The fundamental challenge: Realizing “inverse analysis”

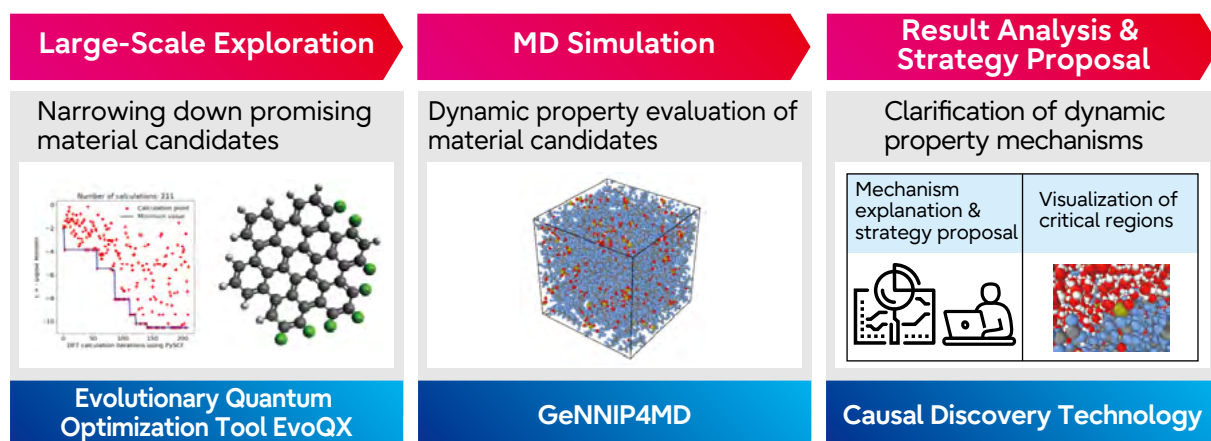
“The fundamental challenge for MI lies in achieving ‘inverse analysis’—determining the conditions required to achieve a new material's desired properties” states Manabu Mizobuchi of Fujitsu's Global Solutions Business Group.

Traditional materials development has typically adopted a “forward analysis” approach: first, defining the material's structure, composition, and process conditions, and then predicting what properties will result. In contrast, inverse analysis reverses this process. It begins by defining the desired properties and then systematically unravels the various conditions required to achieve them. This approach significantly enhances the efficiency of exploring and identifying materials with target properties, leading to reduced development time and costs, and potentially greater precision in material design. Mizobuchi emphasizes, “Fujitsu's strength lies in its ability to independently implement a material creation workflow that integrates computing technology and AI to handle inverse analysis.”

### ■ Overall picture of Fujitsu's MI technologies

A simplified overview of Fujitsu's MI-related technologies is presented below (Figure 4). The combination of large-scale exploration, molecular dynamics (MD) simulations, and result analysis and strategy proposal accelerates the materials development process. Fujitsu optimally integrates AI, computing technology, and robust data infrastructure into this entire process to deliver solutions tailored to each client's specific challenges.

**Figure 4: Advancing the materials development process through multiple technologies**



(Source: Fujitsu)

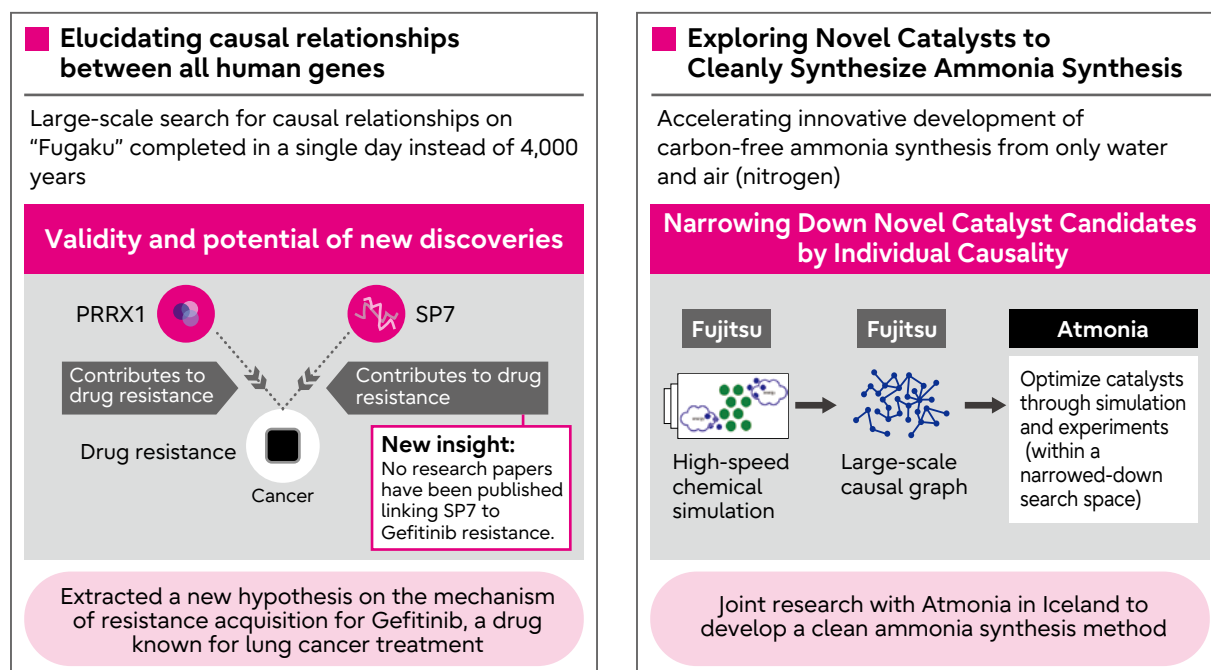
EvoQX is a technology that efficiently discovers “optimal solutions” by combining data learning, quantum-inspired technologies such as the Digital Annealer, and genetic algorithms. Data learning identifies patterns and characteristics of “good solutions” from data and simulations. Quantum-inspired technologies incorporate concepts like “parallelism” and “superposition” from quantum computing, enabling the simultaneous exploration of multiple candidate solutions from vast search spaces and the discovery of elusive optimal solutions. Genetic algorithms gradually improve solution quality by generating multiple candidate solutions, evaluating them, and retaining the most promising ones.

**GeNNIP4MD** (Generator of Neural Network Interatomic Potential for Molecular Dynamics, currently under development) is a tool for generating Neural Network Potentials (NNPs). NNPs are gaining significant attention as a technology that substantially enhances the accuracy and computational efficiency of MD simulations. However, building NNPs typically demands advanced expertise and considerable time, and maintaining stability and accuracy in long-duration simulations remains a challenge.

GeNNIP4MD overcomes these limitations by actively sampling unstable structures and incorporating them into NNP training data, thereby significantly improving the stability of long-duration simulations. Yasufumi Sakai of Computing Laboratory, Fujitsu Research notes, “When applied to the polymer electrolyte membrane of fuel cells, it allowed for over 30 nanoseconds of MD simulation for a 20,000-atom system in just 8 days. This is 100 to 200 times faster than other existing technologies.”

Causal discovery technology is instrumental in eliminating the “black box” in materials development. Fujitsu provides technologies for AI-driven causal discovery and explanation via the research and development version of its cloud-based AI platform, “Fujitsu Kozuchi.” In research on lung cancer treatment, combining AI with the supercomputer “Fugaku” achieved a large-scale causal exploration of all 20,000 genes in just one day, a task that would conventionally take 4,000 years. Furthermore, in collaboration with Atmonia of Iceland, Fujitsu is actively developing new catalysts for cleaner ammonia synthesis (Figure5).

**Figure 5: Discovering critical causal relationships within vast data for specific conditions**

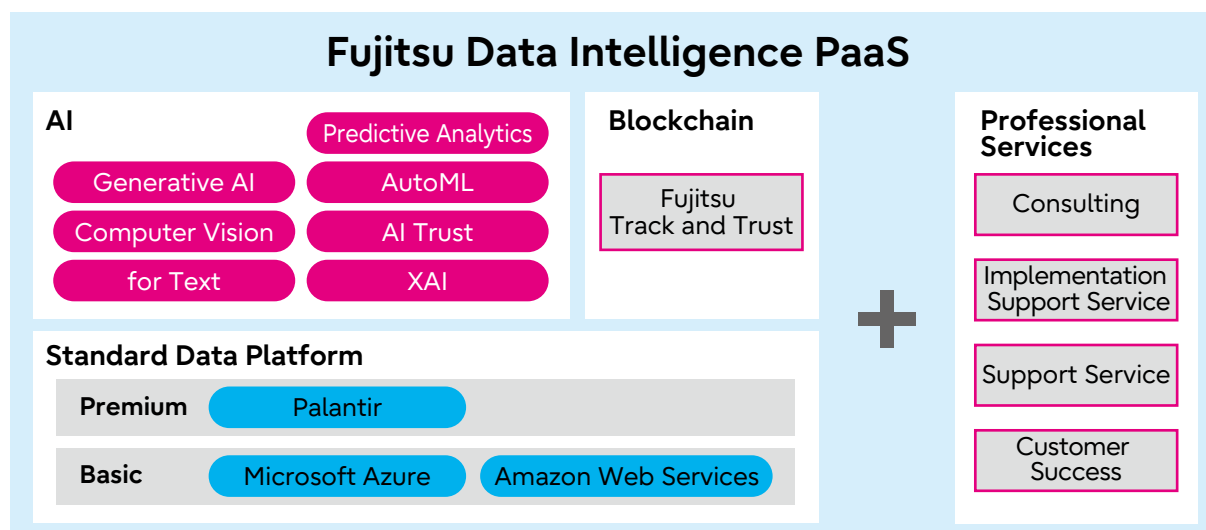


(Source: Fujitsu)

## ■ Integrating AI and blockchain technology into the data infrastructure

For data infrastructure, organizations can leverage Fujitsu Data Intelligence PaaS (DI PaaS), a cloud-based, all-in-one operational platform that integrates extensive, dispersed data from both internal and external sources into an understandable format to support decision-making (Figure 6). DI PaaS facilitates the integration of all relevant data—including R&D information such as experimental data, papers, and patent data, as well as product and production information like costs, design, and manufacturing details. By visualizing this integrated data, it enables efficient searching, analysis, and simulation, thereby empowering informed decision-making.

**Figure 6: Key components of DI PaaS**



(Source: Fujitsu)

## ■ Driving “readiness for technological innovation” and “business, organizational, and human capital transformation”

MI transformation is rapidly accelerating through continuous technological innovation, with quantum computing serving as a prime example. As the pace of change intensifies, breakthroughs in major technological innovations are set to occur with increasing frequency. To optimally harness cutting-edge technologies for business growth when opportunities arise, it is paramount to thoroughly prepare for technological innovation today. Fujitsu commits to partnering with its customers on this journey: collectively envisioning the desired future, backward-designing from that future to identify effective technologies, and steadily advancing step-by-step while solidifying foundational capabilities.

Furthermore, it is crucial to recognize that MI transformation extends beyond mere technology adoption. It fundamentally requires transforming people, organizational structures, and operational processes that underpin technology. This includes integrating and streamlining everything from experimental planning to data analysis and feedback into manufacturing processes digitally. It also involves dismantling data silos to establish mechanisms for sharing knowledge and data across the entire organization and fostering a corporate culture that embraces continuous challenge over adherence to precedent. The key to success lies in implementing optimal technologies in conjunction with a company-wide transformation that maximizes their utilization. This requires consistent execution, prioritized and aligned with the company’s specific challenges.

Past successes can become present obstacles, opportunistic habits can delay reform, and half-hearted adaptation can lead to future failures. All transformations, including MI, are susceptible to such pitfalls. Strong leadership from top management is indispensable for navigating and avoiding these traps that lie hidden within the transformational journey.

## Section 5

# Conclusion

All enterprises today are called upon to view the pervasive global uncertainty not merely as a risk, but as a strategic opportunity for transformation and growth. Materials Informatics (MI) transformation undoubtedly stands as one of the essential strategies to thrive in this era of uncertainty and achieve sustainable growth.

We are now faced with a pivotal choice. Will we remain constrained by the “recipes” of past experience?

Or will we actively pursue the objective truths of “principles”? Taking the decisive step toward a company-wide transformation—encompassing technology, business processes, organization, human capital, and corporate culture—to realize an envisioned future, will lay the essential foundation for creating sustainable new value for generations to come. Hesitation will swiftly erode competitive advantages. The path forward is clear. Let us embark together on this journey to unlock new frontiers in materials development.

## Profile



### Daisuke Suzuki

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Daisuke Suzuki joined Fujitsu in March 2024, following roles at Nikkei Inc. and PwC Japan. At Nikkei Inc., he spent approximately 18 years as a staff writer and editor, covering policy at central government agencies such as the Ministry of Finance, Financial Services Agency, and Ministry of Economy, Trade and Industry, as well as industries including energy and startups. At PwC Japan, he led the planning, editing, and writing of Thought Leadership content as a Manager. He assumed his current position in April 2025.

The author extends deep gratitude to Dr. Yasufumi Sakai, Dr. Hideyuki Jippo, Dr. Hiroyuki Higuchi, and Mr. Manabu Mizobuchi for their insightful review and invaluable advice during the preparation of this insight paper. Sincere appreciation is also expressed to Mr. Takashi Shinden and Ms. Hiroko Meguro for their unwavering support.



