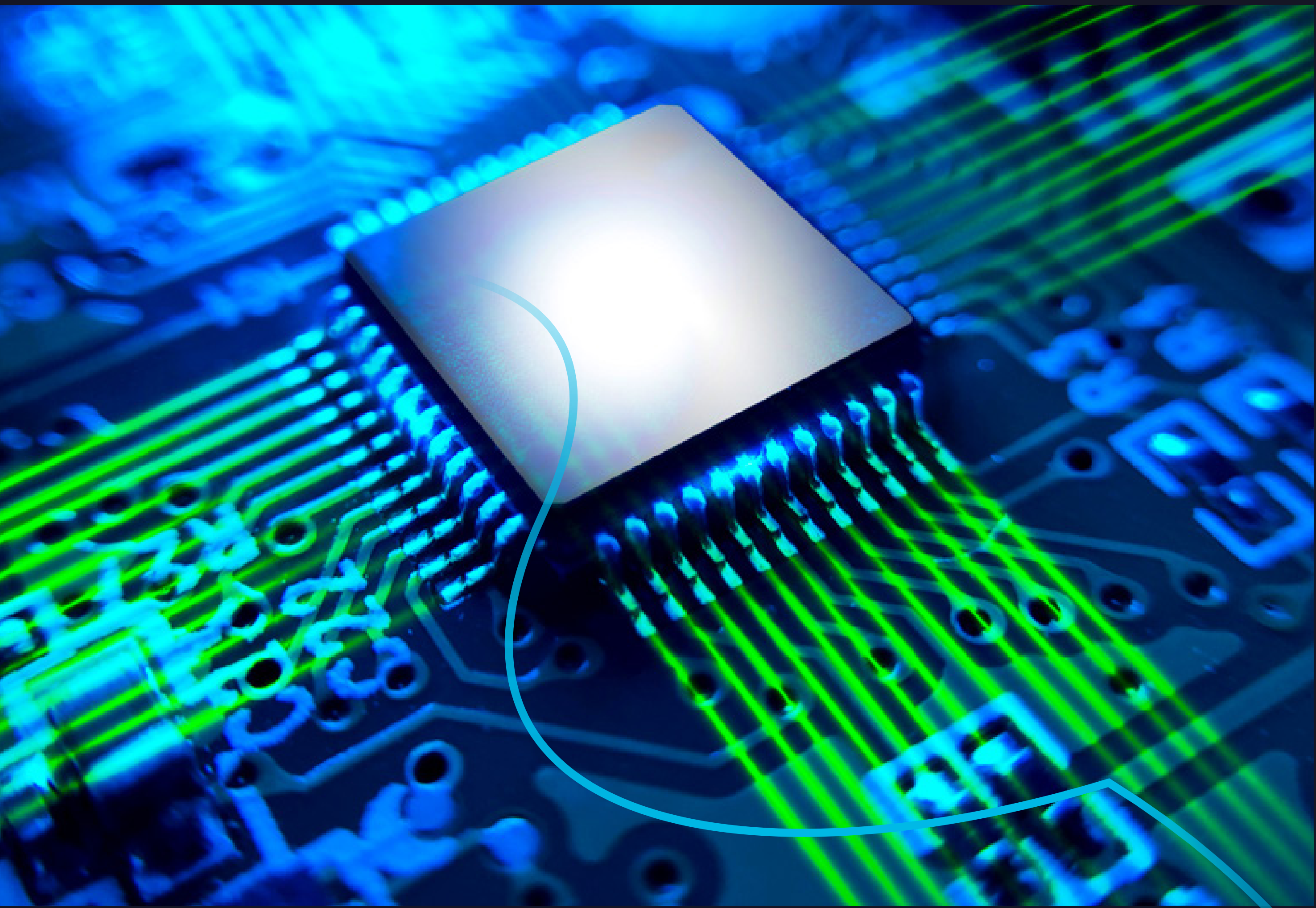
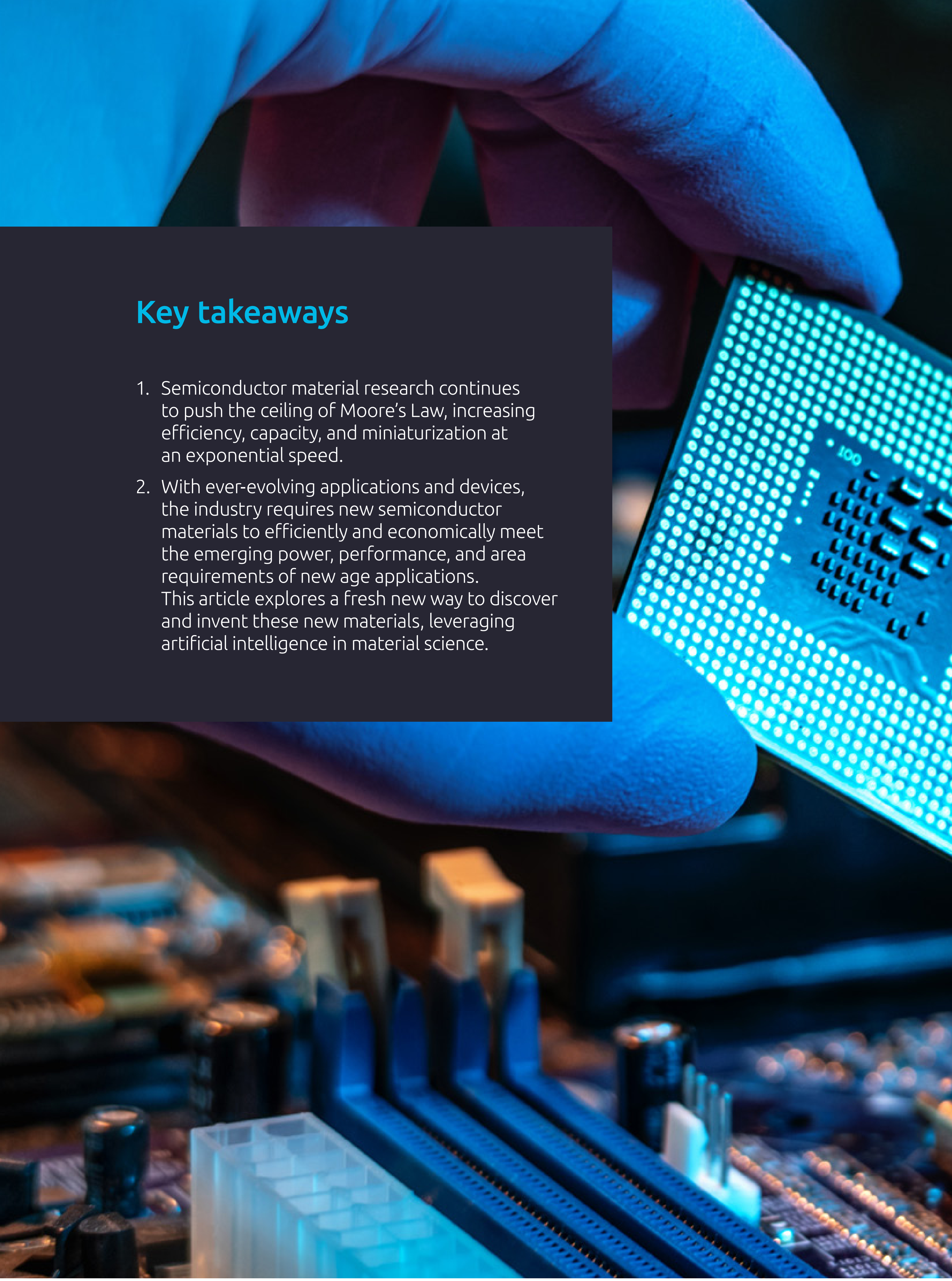


The new and the next for semiconductor materials in the era of generative AI

Capgemini



Key takeaways

1. Semiconductor material research continues to push the ceiling of Moore's Law, increasing efficiency, capacity, and miniaturization at an exponential speed.
2. With ever-evolving applications and devices, the industry requires new semiconductor materials to efficiently and economically meet the emerging power, performance, and area requirements of new age applications.
   This article explores a fresh new way to discover and invent these new materials, leveraging artificial intelligence in material science.

Introduction

Ever wondered how many semiconductor devices we encounter from the time we get up to the time we go back to bed? Almost everything we touch is powered by the smallest, yet most powerful component of that device – the semiconductor! Thus all the technology we use in our daily lives is powered and advanced by constant innovations in the semiconductor industry.

The semiconductor industry has always been uniquely forward-looking. Back in 1965, Gordon Moore mapped the future of the semiconductor industry – before the industry even existed! His predictions have endured to this day, in what's known as *Moore's Law*.

This article will provide a glimpse of the now and next material innovations happening across the semiconductor value chain. Let's take a look at these ever-evolving constituents of semiconductors.

Semiconductor materials – the building blocks of tech

The future of the semiconductor industry looks bright and it's evolving fast. It will be interesting to see the direction the industry heads, but also anxiety inducing, with semiconductors dependent on many factors and innovations. This section examines these factors as they relate to the search for new semiconductor materials.

Traditionally, the three most common semiconductor materials have been *germanium, silicon*, and *gallium arsenide*. Now a few new contenders are throwing their hats in the ring.

Germanium

Germanium, discovered in 1886, is often regarded as the "original" semiconductor. Despite its early promise, it eventually lost favor when manufacturers turned to silicon – a far more abundant and cost-effective alternative. For over six decades, silicon has dominated the semiconductor industry, becoming virtually synonymous with the technology itself.

Lately, however, material scientists have been revisiting germanium for use in transistor technology. The data shows electrons move three times faster in germanium than in silicon,[1] providing an opportunity to improve speed. And with industry experts fearing silicon will soon reach the limits of *Moore's Law*, Germanium just might make a comeback.

Gallium arsenide (GaAs)

Gallium arsenide (GaAs) is the second most widely used semiconductor today. Unlike elemental semiconductors such as silicon and germanium, GaAs is a compound, formed by combining gallium and arsenic. Its eight valence electrons enable rapid response to electrical signals, making it ideal for amplifying high-frequency signals in applications like television satellites. However, GaAs comes with challenges: it is more difficult to manufacture at scale compared to silicon, and its production involves toxic chemicals, raising concerns about sustainability and environmental impact in an already strained semiconductor industry.

Gallium Nitride (GaN)

Gallium nitride (GaN) is emerging as a promising material for next-generation power semiconductors, offering faster and more efficient power conversion in electric grid systems. Its advantages include superior thermal performance, higher efficiency, and reduced weight and size.[2] GaN high electron mobility transistors (HEMTs) have been commercially available since 2005, and many companies are actively developing GaN-based technologies for broader applications.[3]

Silicon Carbide (SiC)

Silicon carbide (SiC) is often compared to traditional bulk silicon, but it offers superior performance for power electronics. Its advantages include higher breakdown voltage, lower energy losses, high-frequency switching capability, and operation at elevated temperatures.[4] These benefits stem from SiC's intrinsic material properties, such as a wider energy bandgap, higher electric breakdown field, and excellent thermal conductivity.

1 Germanium can take transistors where silicon can't, IEEE Spectrum: https://spectrum.ieee.org/germanium-can-take-transistors-where-silicon-cant
2 Driving Cost Lower and Power Higher With GaN, Semiconductor Engineering: https://semiengineering.com/driving-cost-lower-and-power-higher-with-gan/
3 Driving Cost Lower and Power Higher With GaN, Semiconductor Engineering: https://semiengineering.com/driving-cost-lower-and-power-higher-with-gan/
4 Silicon Carbide Vs Silicon: Why SiC is Future of Power Electronics, Electronicsandyou: https://www.electronicsandyou.com/silicon-carbide-vs-silicon-why-sic-is-future-of-power-electronics.html

SiC is currently penetrating markets that require very high current (50 A and above) and voltages exceeding 1700 V, with the potential to support voltages beyond 10 kV. Leading SiC device manufacturers include Wolfspeed, Infineon Technologies, ON Semiconductor, STMicroelectronics, ROHM Semiconductor, General Electric (GE), Fuji Electric, GeneSiC Semiconductor, Mitsubishi Electric, UnitedSiC (Now Qorvo).[5]

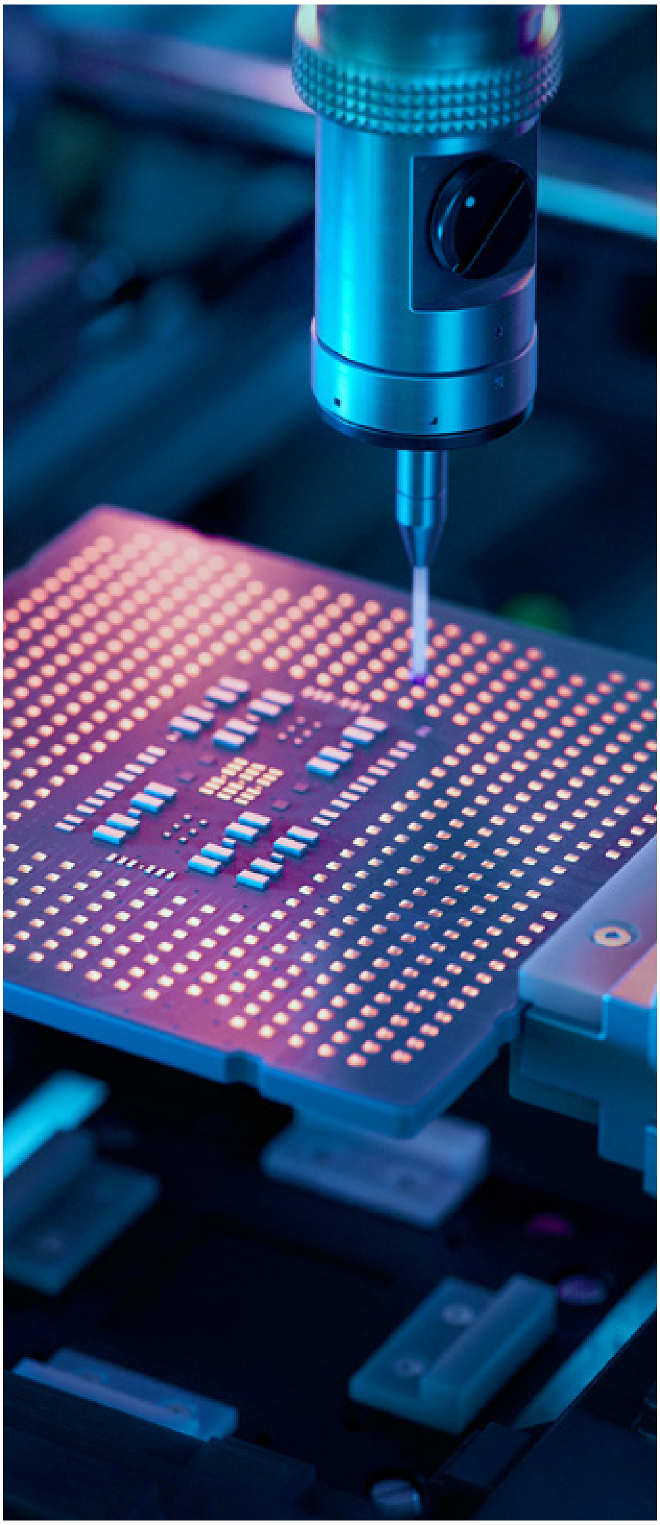
Diamond

Diamond is often hailed as the "ultimate material" for power semiconductor components, frequently mentioned alongside GaN as a wide-bandgap material.[6] It boasts the highest known breakdown strength and exceptional thermal conductivity. However, its wide bandgap also presents challenges, particularly in identifying suitable dopants. Additional technological hurdles – such as inefficient n-type doping, difficulty forming conductive surface channels, and challenges in creating ohmic contacts – have so far prevented the development of high-performance diamond-based devices. Overcoming these barriers will be essential for diamond to play a meaningful role in the future of semiconductor innovation.

Graphene

Graphene is emerging as a strong contender to replace silicon in electronics, thanks to its exceptional strength, flexibility, and conductivity. It's about 200 times stronger than steel and significantly lighter than aluminum, making it ideal for a wide range of industries – from energy and construction to healthcare and tech.

- **Battery Innovation:** Graphene's high conductivity could extend battery life ten-fold[7] and enable much faster charging, potentially replacing many lithium-based batteries.
- **Lightweight Power:** Its low weight and durability make it perfect for drone batteries, where reducing mass is a major advantage.
- **Flexible Tech:** Transparent and ultra-thin, graphene absorbs just 2% of light,[8] making it suitable for bendable screens in phones, TVs, and even cars.
- **Durability in Lighting:** As a tough and efficient conductor, graphene could revolutionize lighting by enabling longer-lasting, energy-saving bulbs that outperform current LED technology.



5 Top 10 Silicon Carbide Semiconductor Manufacturers in the World, Electronicsandyou.com: https://www.electronicsandyou.com/top-10-silicon-carbide-semiconductor-manufacturers-in-the-world.html

6 This Diamond Transistor Is Still Raw, But Its Future Looks Bright, IEEE Spectrum: https://spectrum.ieee.org/this-diamond-transistor-is-still-raw-but-its-future-looks-bright

7 Graphene Jolts Sodium-Ion Battery Capacity, IEEE Spectrum: https://spectrum.ieee.org/graphene-sodium- ion-battery

8 Graphene-Based Nanomaterials And Their Applications, Nature Research Intelligence: https://www.nature.com/research-intelligence/nri-topic-summaries/graphene-based-nanomaterials-and-their-applications-micro-1206

Semiconductor materials research in the new era

Generative AI is impacting the automotive, aerospace, defense, medical, electronics, and energy industries by composing entirely new materials targeting specific physical properties. The process, called inverse design, which defines the required properties and discovers materials likely to have them – infinitely more efficient than relying on serendipity to find the right material. Generative models are well-suited for inverse design tasks, enabling researchers to identify materials that meet specific performance requirements.

A parallel can be seen at the health & drug industry[9] where generative AI is rapidly transforming drug research by accelerating and improving various stages of the drug discovery and development process. Gen AI models can analyse vast datasets, predict molecular properties, identify new drug targets, and even generate novel drug candidates, ultimately speeding up the development of new therapies and potentially saving time and resource.

While Gen AI has the capability to propose new molecules, it typically cannot perform optimization tasks on its own. Effective optimization often requires additional mechanisms, such as reinforcement learning frameworks. These frameworks are essential for evaluating and improving the solutions generated by Gen AI, helping to determine whether they represent actual improvements or not.

Here are some ways how Gen AI is being used in drug research to accelerate drug discovery and development:

Lead Discovery: Gen AI models can be trained to generate novel molecules with desired properties, potentially leading to new drug candidates.

Drug Repurposing: Gen AI can analyze existing drugs to identify potential new uses for them, accelerating the development of treatments for new indications.

Molecular Generation: Gen AI models can generate novel, valid molecules with desired properties, such as binding to a specific receptor.

Optimizing Chemical Processes: Gen AI can assist the optimization of chemical processes involved in drug manufacturing, such as reaction conditions and reaction yields.

9 Inverse design, ScienceDirect: https://www.sciencedirect.com/topics/engineering/inverse-design

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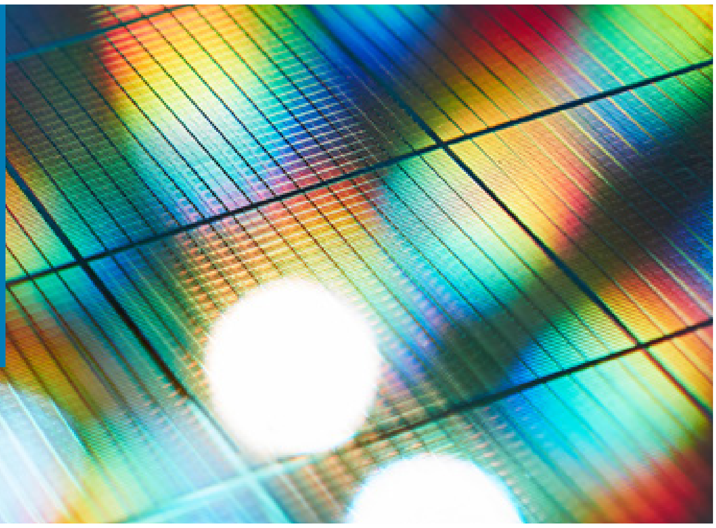

Prospective generative AI models in semiconductor materials science

Like the drug research and development cited above, we foresee similar innovations in Gen AI-based material science research for semiconductors.

The electronics industry constantly seeks new materials with enhanced electrical, thermal and optical properties. Generative models can contribute to the discovery and development of next-generation semiconductor material (both natural and synthetic) which will power the electronic devices with improved performance and energy efficiency.

They can also assist in optimizing existing materials by suggesting modifications to enhance their properties. This capability is particularly valuable in industries where even incremental improvements in material performance can have significant impacts.

Researchers have used generative models to discover new thermoelectric materials with improved performance, paving the way for more efficient energy conversion technologies. For example, the optimization of solar cell materials was based on generative models, and has led to increased efficiency and reduced costs. Now, that same technique is being applied to semiconductor material research. One recent study[10] used Gen AI to explore the properties of Nitrogen-Gallium (N–Ga), Silicon-Germanium (Si–Ge), and Vanadium-Bismuth-Oxygen (V–Bi–O).

Today, Moore's Law is running up against the laws of physics for silicon and germanium. The next generation of semiconductors is on the way, thanks to Gen AI models deeply trained on a vast knowledgebase of material science. Gen AI is helping us discover new materials and recommends component molecules or doping to optimize existing semiconductor materials. This should lead to better performance, lower costs, lower thermals, less energy consumption, and bionic compatibility.

For example, Gen AI can be used to design novel molecules or compounds with better conductivity, thermal stability, gate size, leakage current, or biocompatibility for bionics- based chip design. These new materials can enable new functionalities or applications for semiconductor devices, especially in More-than-Moore use cases. One such great approach paper *"Inverse design for materials discovery from the multidimensional electronic density of states"* describes how to accelerate materials discovery, a deep learning method for inverse design of inorganic materials using multidimensional DOS properties was developed.

10 Inverse design of semiconductor materials with deep generative models, Journal of materials chemistry: https://pubs.rsc.org/en/content/articlelanding/2024/ta/d4ta02872d

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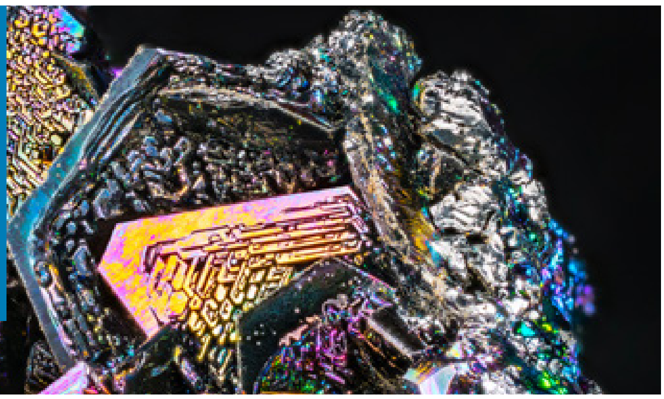
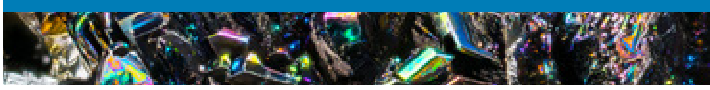
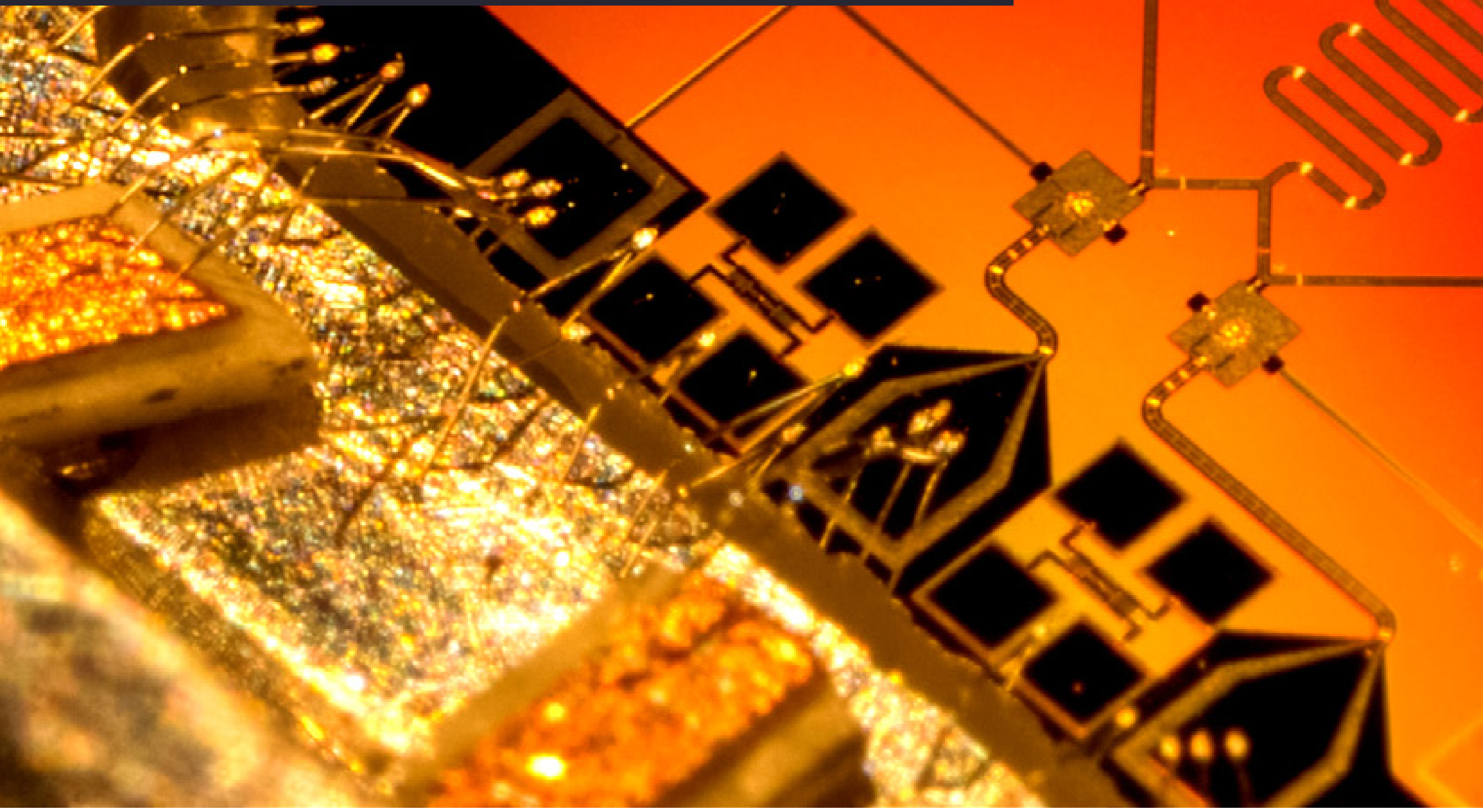
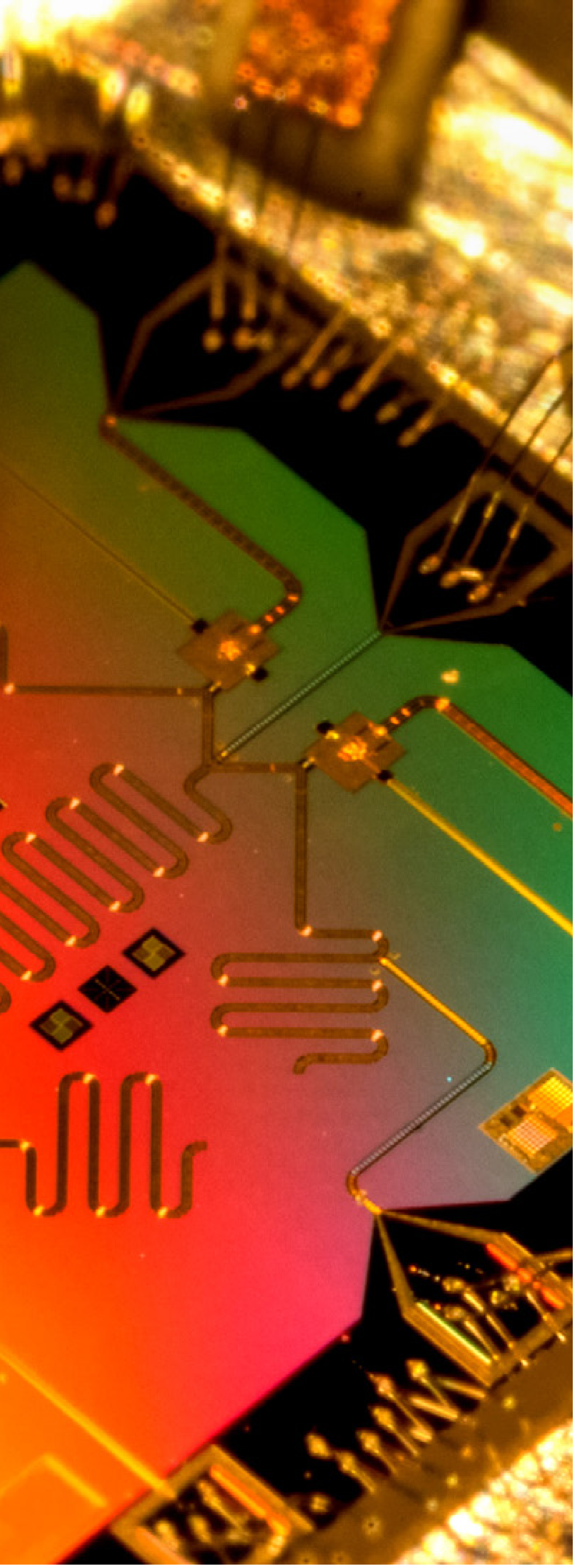




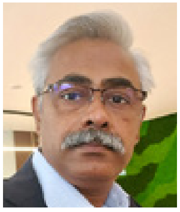
Summary

Generative models are revolutionizing materials science by enabling researchers to design and discover novel materials with unprecedented speed and efficiency. These AI-powered tools are transforming the materials discovery process, from novel materials design to property prediction and optimization, so in principle we are looking at some big advantages in reducing time to discovery. However: the ultimate test of any new material is its performance in real-world applications. Efficient experimental validation processes are necessary to bridge the gap between computational predictions and practical implementation.





About the author



Ravi Gupta
Senior Director
Industry and Innovation
Capgemini
ravi.b.gupta@capgemini.com

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