What's next in materials science?

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The Innovation Materials (TIMS), launched on June 27, 2023, is a sister journal of *The Innovation*, dedicated to disseminating cutting-edge ideas, research breakthroughs, and real-world applications in materials science.[1] Over the past three years, with steadfast support from our editors, editorial board members, authors, readers, staff, and cover art contributors, TIMS has demonstrated strong momentum in sharing the latest scientific discoveries and technological advances—evidenced by its latest Scopus CiteScore Tracker 2025 (9.9, updated January 6, 2026). As TIMS enters its fourth year, we would like to share perspectives on the theme "What's next in materials science" (Figure 1), aiming to fuel the vibrant growth of materials science and related fields. Notably, this editorial is part of the "What's Next in XX Science" series launched by *The Innovation*, and will be featured across our sister journals.

COMPLEXITY OF MATERIALS

The frontier of materials science has shifted decisively from describing static structures to engineering the dynamic, multi-scale interactions that dictate functionality. This paradigm necessitates the convergence of advanced characterization, a new design philosophy, and synthetic methods that deliberately harness complexity. Functional properties emerge from the synergistic interplay of features across all scales, from atomic defects and interfaces to microstructural architectures. To decode these relationships, characterization has evolved to include in situ and operando techniques such as four-dimensional scanning transmission electron microscopy,[2] which provides concurrent, real-space mapping of atomic structure, strain, and electromagnetic fields. Complementing this, precise atomic-scale manipulation and controlled multi-scale assembly are now essential, while artificial intelligence integrates multimodal data into predictive, physics-informed models. Complexity itself has become a foundational design parameter.

Material science is shifting from pursuing perfect structures to intentionally engineering complexity, treating disorder and imperfections as design parameters. For instance, high-entropy alloys and ceramics exploit configurational entropy and severe lattice distortion to stabilize unprecedented phases with unique combinations of properties. Defect engineering enables the deliberate modulation of vacancies, dislocations, and grain boundaries to tailor ionic transport, catalytic activity, and mechanical response. The overarching aim is to orchestrate entropy stabilization, size effects, and interfacial phenomena into material systems characterized by "controlled imperfection". This refined understanding enables a new generation of adaptive and programmable functional materials. For quantum materials and those operating in extreme environments, it demands atomically precise control over electron correlations and defect dynamics under harsh conditions. The trajectory points toward programmable matter: by integrating responsive components into architectured frameworks—such as 3D micro-lattices or kirigami-inspired metamaterials—or by using external fields to dynamically reconfigure internal order parameters, materials can be designed to adapt, switch properties on demand, or execute logic-like functions. This new paradigm, powered by integrated multi-scale insight and computational design, is transitioning the field from empirical discovery to the on-

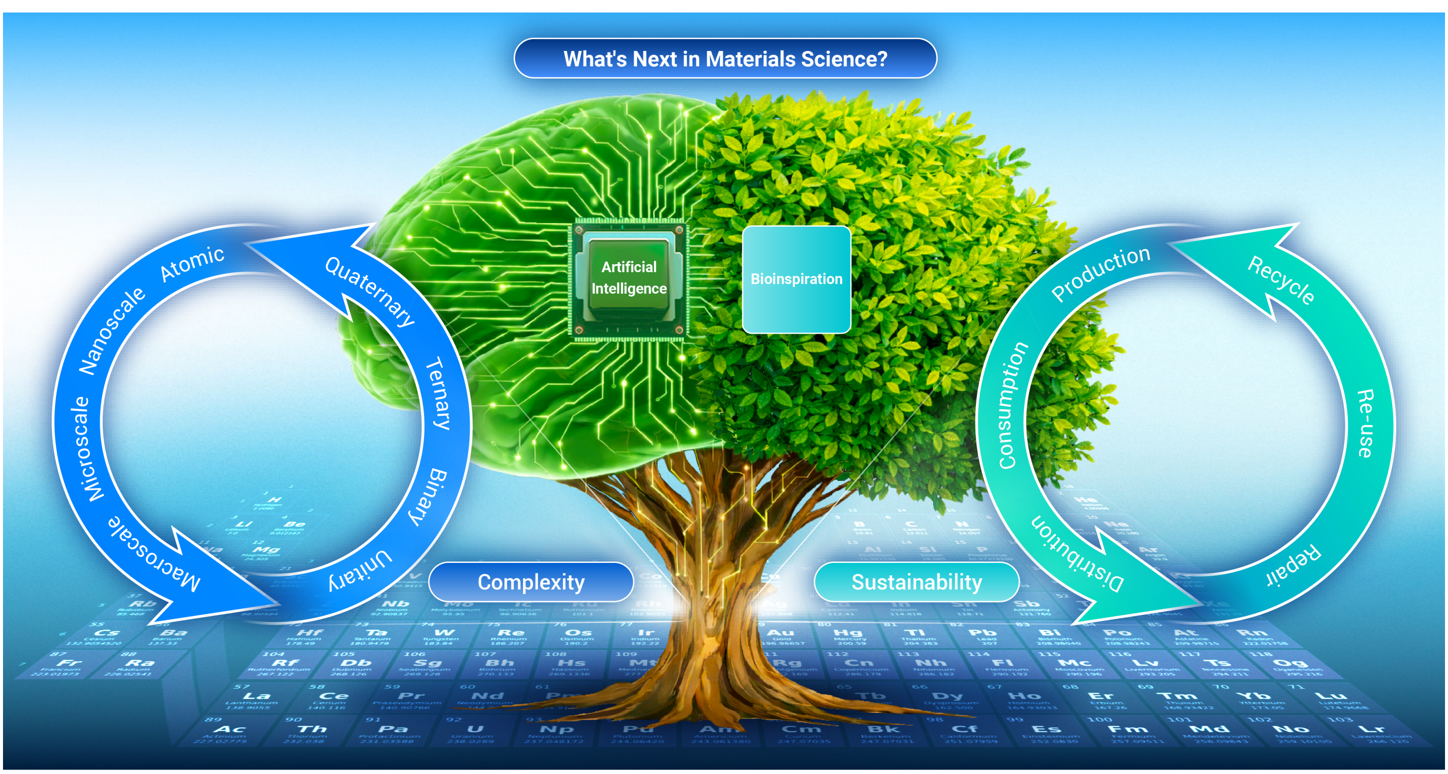

Figure 1. Artificial intelligence and bioinspiration drive advances in materials science.

demand creation of material systems with tailored, dynamic, and intelligent functionality.

SUSTAINABILITY FOR MATERIALS

The 21st-century materials science is no longer simply delivering superior performance in areas like strength or conductivity. It now requires achieving such performances within the strict confines of planetary sustainability.[3] This paradigm shift demands that environmental and social impact become primary design criteria, guiding material innovation from the laboratory to the global scale.

The traditional focus on the "use phase" of a material is now expanding to encompass its entire life cycle. This means that materials are intentionally designed from the outset to enable biodegradability, recyclability, and low-carbon synthesis pathways. A key challenge is the dependence on metals and fossil feedstocks whose supply chains are concentrated and unstable. The clean energy transition, for instance, hinges on critical metals such as lithium, cobalt, and rare earth elements, which have vulnerable supply chains. Research now prioritizes materials with abundant and renewable constituents, substitutes for critical elements, and designs that facilitate End-of-Life recovery. Computational tools like materials informatics and artificial intelligence (AI) are also being used to screen for such sustainable candidates early in the discovery process.

The manufacturing process for materials is undergoing a green revolution. This involves developing bio-based polymers from renewable feedstocks such as lignocellulosic biomass, employing green catalysis to reduce toxic byproducts, and pioneering low-energy processes, such as low-temperature synthesis. Such a "green chemistry" pathway aims to prevent pollution and carbon emissions at the source. Concurrently, the vision of a circular economy is being materialized through advanced recycling technologies. "Urban mining" to extract valuable elements from electronic waste and novel chemical recycling methods that break down plastics into their original monomers are moving from concept to pilot scale. For example, chemical recycling of polyethylene terephthalate offers a promising path to achieve excellent recyclability with minimal quality loss. The combination of non-grain biomass-based materials, low-energy processes, and scalable waste-recovery techniques will embed sustainability into manufacturing.

Materials science is the cornerstone of the energy transition. Accelerated material innovation is crucial in next-generation batteries, new photovoltaics, hydrogen energy, and grid-scale energy storage. Each leap in efficiency, durability, or cost reduction in these areas directly accelerates decarbonization. Sustainability has evolved from a constraint into a powerful catalyst for innovation in materials science, and continued interdisciplinary innovation is essential to build a carbon-neutral future. Thus, the integrated pursuit of life-cycle design, green synthesis, and energy materials creates a virtuous cycle. The future lies in smart materials designed with their end of life in mind, manufactured through benign processes, and deployed to build a negative-emission civilization. This holistic approach positions materials scientists not only as creators of substances but also as architects of a sustainable future.

LEARNING FROM AND INTEGRATING WITH NATURE

Given the complexity of materials and the demand for sustainability, learning from and integrating with nature provides a paradigm for materials science: from observing nature to deeply learning from it, and finally to integrating biological principles into the very fabric of our material designs. This evolution is catalyzing the emergence of a sophisticated field centered on nature as the Ultimate Materials Designer. Over billions of years, evolution has engineered biological systems with extraordinary capabilities—unmatched strength-to-weight ratios, inherent toughness, dynamic adaptability, and self-repair.[4] These properties are encoded in sophisticated architectures: the layered fortitude of nacre, the hierarchically porous and graded structure of bone, and the precise protein assembly of spider silk. Today, we are decoding these biological blueprints to create synthetic materials that not only match but often seek to surpass these natural benchmarks.

This foundational insight propels us toward a critical frontier: Bio-Inspired Manufacturing and Multifunctionality. The objective extends beyond mimicking static forms to mastering dynamic processes and achieving integrated, system-level functions. This approach is generating novel material concepts—such as programmable hierarchical and gradient structures, and responsive networked materials—that translate into transformative applications. We see this in the compliant, adaptive actuators of soft robotics; in smart surfaces endowed with self-cleaning or drag-reducing properties inspired by plant leaves and shark skin; and in the development of advanced biocompatible materials designed for seamless synergy with living tissues.

This confluence of learning from and integrating with nature is redefining the horizons of materials science. It steers the field toward creating next-generation material systems that are not merely high-performing, but also adaptive, responsive, and inherently sustainable. Contributing to this vibrant discourse and sharing discoveries that bridge biological wisdom with engineering innovation would shape a more resilient and intelligent material future.

AI-DRIVEN PARADIGMS IN MATERIALS SCIENCE

The integration of AI is reshaping materials science, shifting the field from traditional, often serendipitous, experimentation towards an intelligent, data-driven, and predictive discipline. This transformation is establishing new paradigms that accelerate the discovery, design, and deployment of advanced materials.[5]

Historically, materials discovery relied heavily on intuition and costly trial-and-error. AI is revolutionizing this process by extracting complex patterns from vast datasets. Techniques such as material graph neural networks and large language model trained on scientific literature enable the prediction of material properties at an unprecedented speed. Knowledge graphs further integrate disparate data, uncovering hidden relationships. This data-centric approach is amplified by high-throughput computation and experimentation, which generate the necessary training data. The ultimate expression of this trend is the emergence of autonomous "self-driving labs," where AI algorithms plan, execute, and analyze experiments in a closed loop, dramatically accelerating the research cycle.

Moving beyond property prediction, generative AI models enable an inverse design paradigm. Instead of screening known materials for a desired property, models can now generate entirely novel atomic structures, molecular compositions, or microstructures tailored for specific applications, such as, high-efficiency catalysts, next-generation battery electrolytes, or complex crystalline phases. This represents a shift towards a true design-to-device philosophy, where materials are engineered from the ground up to meet the exact requirements of a final application, streamlining the path from laboratory innovation to functional technology.

Despite its promise, this AI-driven transition faces significant hurdles. Key challenges include the scarcity and heterogeneity of high-quality materials data, the "black-box" nature of many complex models that limit interpretability, and the difficulty of cross-scale modeling that bridges atomic interactions to macroscopic behavior. Furthermore, the rise of AI raises critical questions regarding research norms, intellectual property, and ethical use of automated systems. It also pressures traditional academic publishing and peer-review models to adapt to AI-assisted research. Addressing these challenges is essential to fully harness AI's potential to usher in a new era of efficient, intelligent, and innovative materials science.

In summary, complexity and sustainability are emerging as defining frontiers for the future of materials science. Learning from nature and adopting AI-driven discovery offer two powerful paradigms that transform the field from empirical trial-and-error to predictive design and intelligent fabrication of high-performance yet sustainable systems. By integrating biological principles with computational capabilities, materials scientists are poised to create next-generation materials that are not only adaptive and intelligent but also aligned with planetary boundaries, thereby paving the way to a carbon-neutral future.

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DECLARATION OF INTERESTS

The authors declare no competing interests.