

Smart, Sustainable, and Advanced materials for the 21st century

Author (s): Dr. Ravi Kashikar, Vidyashree Hebbar

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Human civilization has witnessed an exponential increase in innovation quality, enabling humankind to evolve toward greater efficiency and creativity. Unlike previous centuries, the 21st century, although only a quarter has been completed, has already experienced transformative advancements in technology and lifestyle. This accelerated evolution is largely attributed to the rate of innovation and the increasingly material-centric approach to technological development. Throughout history, materials have played a crucial role in shaping civilization, starting from natural substances to reaching engineered composites. Metals like iron have been known for 3000 years; however, the meticulous design of iron-carbon alloys, i.e., steel, has revolutionized global infrastructure and industrialization [1]. The curiosity of researchers about the structure, properties, and manipulation of matter is the driving force for inventing new materials from time to time.

The nineteenth century, often called the age of the industrial revolution, centred largely on the mastery of structural materials and the large-scale refinement of naturally occurring compounds. The defining achievement was the advancement of ferrous metallurgy. Suddenly, strong, affordable steel was available in unprecedented quantities, forming the literal backbone of modern infrastructure. This abundance enabled the construction of towering skyscrapers, long-span bridges, and expansive railway networks, fundamentally altering urban design, manufacturing, and global transportation [2]. The twentieth century inaugurated the age of synthetic materials,

fundamentally shifting the focus from purifying metals to synthesizing complex organic and inorganic compounds with specific, predetermined properties. The 20th century was primarily driven by two massive forces: the chemical industry's growth and the emergence of electronics. The breakthrough moment was the creation of Bakelite in 1907 by Leo Baekeland, the first truly synthetic plastic that was non-conductive, heat-resistant, and moldable, effectively launching the polymer age. Throughout the century, subsequent synthetic polymers, including Nylon, Teflon, and Polyethylene, became famous, replacing traditional materials like glass, wood, and metal in thousands of applications, from textiles and cookware to packaging and medical devices [3]. Furthermore, the development of high-performance materials, such as Kevlar in the 1960s, demonstrated that synthetic design can surpass the tensile strength of steel, opening new protective applications in defense and safety equipment [4]. This synthetic revolution allowed engineers to specify attributes like flexibility, chemical inertness, and lightweight durability.

The latter half of the 20th century was defined by the discovery and refinement of semiconductors, particularly pure crystalline silicon. The invention of the transistor in 1947, built upon these precisely manufactured materials, was arguably the single most important material innovation of the era, enabling the miniaturization and mass production of integrated circuits [5]. This electronic step established the foundation for modern computing, telecommunications, and the entire digital revolution. In addition, the demands of the cold war, the space race, and jet propulsion also drove the development of Advanced Metal Alloys like highly durable superalloys (e.g., nickel-based alloys for turbine blades) and lightweight, high-strength titanium alloys. In the mid-20th century, the optimization of natural materials had reached its limit, and there were scope for further optimization. This led to a paradigm shift toward the design of synthetic materials that permit control at the atomic and molecular scales [6].

The transition between 20th and 21st centuries marked a major milestone, as advancements in theoretical modelling, computational simulations, and experimental methodologies enabled the atomistic engineering of both inorganic and organic

systems. These efforts have resulted in the emergence of advanced materials. These materials are engineered substances with tailored properties optimized for specific applications. Over the past three decades, such materials have demonstrated remarkable potential, leading to significant breakthroughs in high-technology sectors including electronics, energy storage, medical diagnostics, and sustainable manufacturing. One of the prominent materials of this century is Graphene, a single atomic layer of carbon atoms, discovered in 2004. It is the thinnest, strongest, and most conductive material known, promising a revolution in flexible electronics, energy storage, and ultra-filtration [7]. The creation of other 2D materials and nanomaterials like Carbon Nanotubes (CNTs) demonstrates a newfound ability to exploit quantum mechanics and high surface area effects for technological gain. Furthermore, the 21st century is heavily characterized by a drive toward sustainability and solving global challenges in energy and health. This has led to the rapid development of Perovskites for solar power. Unlike oxide perovskites, halide perovskites are cheap, highly efficient, and easily processed materials that could soon disrupt the silicon photovoltaic market [8]. The Metal-Organic Frameworks (MOFs), which got the 2025 Nobel prize in chemistry, are porous crystalline structures engineered for highly efficient gas separation, carbon capture, and clean energy storage [9]. Research and development of new advanced materials for industrial applications is multi-disciplinary and can draw on expertise in the fields of chemistry, physics, nanotechnology, ceramics, metallurgy, and biomaterials. Figure 1 illustrates the various categories of advanced materials [10].



Fig.1: Broad classification of advanced materials by German Environment Agency (Ref. Source: Environ. Sci.: Adv., 2023, 2, 162)

The interdisciplinary approach of materials science, nanotechnology, and computational design is reshaping the boundaries of 21st-century innovation. In the upcoming years, advanced materials are expected to fuel substantial economic growth, as depicted in Figure 2 based on analyses by Market.us News.

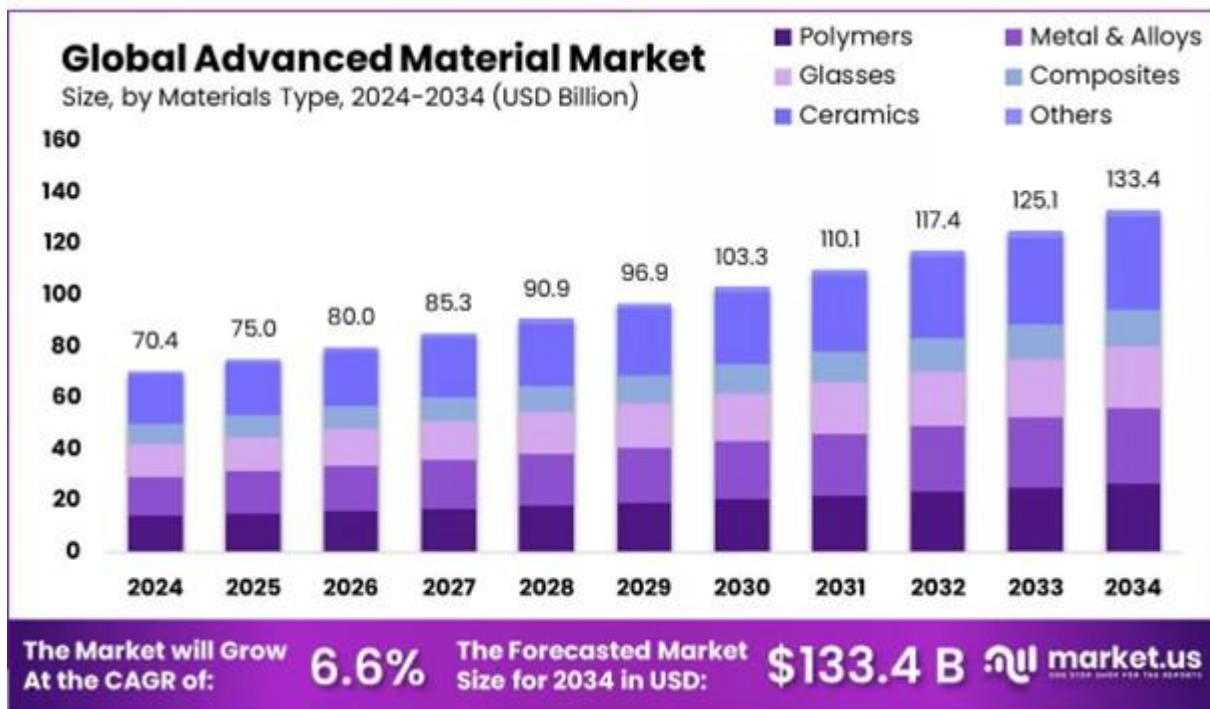


Fig.2: Growth of the Advanced materials market in the USA in the upcoming years. The image is obtained from <https://www.news.market.us/advanced-material-market-news>

The following sections are organized according to the key properties of materials, and we elaborate on how recent material discoveries are shaping the futuristic applications. The broad categories considered are:

- Energy storage materials
- Energy conversion materials
- Electronic materials

Energy storage materials

Energy storage materials lie at the heart of modern energy technologies and play an important role in facilitating the global transition toward renewable and sustainable energy systems. As the world moves away from fossil fuels, the demand for efficient, high-capacity, and durable energy storage solutions has grown tremendously. In response, extensive research has focused on developing advanced materials for

batteries, supercapacitors, and hydrogen storage systems to meet the increasing energy and environmental challenges. Lithium-ion batteries (LIBs) continue to dominate the market due to their high energy density, long cycle life, and reliability [11]. However, innovations in electrode and electrolyte materials are revolutionizing their performance. Advanced anode materials such as graphite and lithium titanate ($\text{Li}_4\text{Ti}_5\text{O}_{12}$), and cathode materials including LiCoO_2 , NMC (LiNiMnCoO_2), NCA (LiNiCoAlO_2), LiFePO_4 , and LiMnPO_4 , are being optimized to enhance capacity, stability, and safety. Emerging concepts like solid-state electrolytes, silicon anodes, and lithium-sulfur (Li-S) and lithium-air (Li-air) batteries promise even higher energy densities and improved safety profiles [12]. Although Li-S and Li-air systems offer exceptional theoretical energy densities and utilize abundant materials such as sulfur and oxygen, they still face challenges like poor cycle life, capacity fading, and significant volume expansion during repeated charge-discharge cycles.

Beyond lithium-based systems, sodium-ion and magnesium-ion batteries are being actively explored as sustainable and cost-effective alternatives, owing to the abundance and low cost of sodium and magnesium compared to lithium. In the realm of supercapacitors, materials such as graphene, carbon nanotubes (CNTs), and metal-organic frameworks (MOFs) have significantly improved charge storage capacity, energy density, and cycling stability. Current research trends focus on hybrid supercapacitors, which aim to combine the high power density of conventional supercapacitors with the high energy density of batteries [13].

Furthermore, redox flow batteries are gaining increasing attention due to their scalability, long cycle life, operational safety, and cost-effectiveness, making them ideal for grid-scale applications. In parallel, advancements in hydrogen storage materials, including metal hydrides and porous frameworks, are accelerating the adoption of hydrogen as a clean fuel [14].

Energy conversion materials

The 21st century has witnessed an unprecedented demand for clean, efficient, and sustainable energy technologies. As the global community transitions toward renewable energy systems, the development of functional materials capable of

converting solar, thermal, chemical, or mechanical energy into electricity with high efficiency and minimal environmental impact has become central to scientific and technological progress. These advanced materials form the foundation of modern energy innovation, enabling the design of systems for energy generation, conversion, and storage that are both environmentally benign and economically viable.

Among the most remarkable advancements are photovoltaic materials, particularly metal halide perovskites such as $\text{CH}_3\text{NH}_3\text{PbI}_3$ (MAPbI_3), FAPbI_3 , and mixed-halide variants like $(\text{CsPb}(\text{Br}_x\text{I}_{1-x})_3)$. These compounds have transformed the solar energy landscape due to their exceptional power conversion efficiencies exceeding 25%, combined with solution-processability, tunable band gaps, and low-cost fabrication methods. Unlike traditional silicon (Si) and cadmium telluride (CdTe) solar cells, perovskite-based photovoltaics can be fabricated on flexible substrates and integrated into tandem architectures with silicon to surpass the Shockley–Queisser efficiency limit. Current research efforts are focused on enhancing their moisture and thermal stability, developing lead-free compositions such as Sn-based perovskites ($\text{CH}_3\text{NH}_3\text{SnI}_3$), and improving scalable deposition techniques including spin coating, blade coating, and vapor-assisted processing for large-area applications[15].

Parallel progress in photocatalytic materials has opened up new avenues for solar-driven hydrogen production and carbon dioxide reduction, which are essential for achieving carbon neutrality and sustainable fuel generation. Prominent photocatalysts such as titanium dioxide (TiO_2), graphitic carbon nitride ($\text{g-C}_3\text{N}_4$), bismuth vanadate (BiVO_4), and zinc oxide (ZnO) have been extensively studied for their chemical stability and photoactivity [16]. To enhance light absorption and charge separation, these materials are often modified through metal or non-metal doping (e.g., N, S, Fe), heterojunction engineering (such as $\text{TiO}_2/\text{g-C}_3\text{N}_4$ composites), or plasmonic coupling using Au or Ag nanoparticles. Such modifications enable better utilization of visible light and higher catalytic efficiency, promoting sustainable routes for hydrogen generation and CO_2 conversion into useful hydrocarbons.

Another major class of energy materials includes thermoelectric materials, which directly convert waste heat into electricity based on the Seebeck effect. Recent

advances in nanostructuring, defect engineering, and alloying strategies have significantly improved their performance by enhancing the Seebeck coefficient, increasing electrical conductivity, and reducing lattice thermal conductivity. Classical materials such as bismuth telluride (Bi_2Te_3) and lead telluride (PbTe) continue to serve as benchmarks for near-room and high-temperature applications, respectively. Meanwhile, silicon–germanium (SiGe) alloys and skutterudites (CoSb_3) have emerged as high-performance materials for waste heat recovery in automotive, aerospace, and industrial sectors. Recent efforts also focus on half-Heusler compounds and oxide-based thermoelectrics (e.g., $\text{Ca}_3\text{Co}_4\text{O}_9$, SrTiO_3) due to their abundance, stability, and environmental compatibility [17].

Electronic Materials

The field of advanced electronic materials is driving the next wave of technological innovation, moving beyond the physical limitations of traditional silicon-based electronics. Research is focused on materials that offer superior performance, smaller size, greater energy efficiency, and novel functionalities for applications like artificial intelligence, quantum computing, and flexible devices. The first quarter of this century has witnessed many advanced electronic materials, such as 2D Materials, Quantum Materials, and Halide perovskites for optoelectronics.

Two-dimensional (2D) materials, composed of atomically thin layers only one atom thick, represent one of the most exciting frontiers in modern materials science and nanotechnology. Their extraordinary structural, electrical, and optical properties have positioned them as potential alternatives or supplements to conventional silicon-based materials that currently dominate the electronics industry. Among them, graphene has attracted unparalleled attention and is often referred to as the “wonder material” of the 21st century. It exhibits exceptional mechanical strength, being about 200 times stronger than steel, while remaining incredibly lightweight and flexible. Moreover, its electrical conductivity surpasses that of copper by nearly 13 times, making it a leading candidate for next-generation high-speed transistors, flexible electronic devices, and ultra-broadband communication systems [7].

In addition to graphene, transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS_2) are atomically thin semiconductors that offer a controllable bandgap, which is essential for fabricating nanoscale transistors and optoelectronic devices. These materials can help overcome the miniaturization limits faced by traditional silicon-based components [18]. Another emerging class of 2D materials, MXenes, are composed of transition metal carbides and carbonitrides. They exhibit a rare combination of metallic conductivity and hydrophilic surface chemistry, making them ideal for applications in transparent conductive films, energy storage devices such as supercapacitors and batteries, and electromagnetic shielding [19].

Beyond these, quantum materials represent the next frontier in condensed matter physics and device innovation. These materials, including topological insulators, Weyl semimetals, and superconductors, exhibit exotic quantum phenomena such as spin-momentum locking, superconductivity, and quantum Hall effects at the nanoscale. Their ability to manipulate electron spin and quantum coherence opens the door to ultra-secure communication, quantum computing, and energy-efficient electronic devices [20]. Furthermore, hafnium oxide (HfO_2)-based resistive random-access memory (RRAM) offers a promising route toward non-volatile memory technologies due to its excellent scalability and compatibility with complementary metal-oxide-semiconductor (CMOS) fabrication processes. Doping HfO_2 with rare-earth elements like lanthanum has shown to enhance its stability and performance in analog and neuromorphic computing [21].

Table 1 summarizes various advanced materials in energy conversion, energy storage and electronic materials



Category	Material	Key Features
Energy Storage Materials	Lithium Iron Phosphate (LiFePO ₄)	Stable olivine structure, thermal safety
	Lithium Nickel Manganese Cobalt Oxide (NMC)	High energy density, tunable composition
	Lithium Nickel Cobalt Aluminum Oxide (NCA)	High energy and power performance
	Silicon–Graphene Composite Anodes	High specific capacity, flexibility
	Solid-State Electrolytes (LLZO, Li ₁₀ GeP ₂ S ₁₂)	Non-flammable, high ionic conductivity
	Sodium-Ion Battery Materials (NaMO ₂ , Prussian Blue)	Abundant, low-cost alternatives to Li-ion
	MXenes (Ti ₃ C ₂ T _x family)	2D conductive carbides/nitrides
	Metal–Organic Frameworks (MOFs)	High porosity, tunable chemistry
	Organic Redox Polymers	Lightweight, flexible, eco-friendly
Energy Conversion Materials	Perovskite Halide Solar Materials (CH ₃ NH ₃ PbI ₃ , etc.)	High power conversion efficiency
	Quantum Dot Materials (PbS, CdSe QDs)	Tunable bandgap, high photoluminescence
	2D Transition Metal Dichalcogenides (MoS ₂ , WS ₂)	Tunable bandgap, photocatalytic activity
	Graphene–Hybrid Systems	High conductivity, transparent
	Cu ₂ ZnSnS ₄ (CZTS)	Earth-abundant, eco-friendly



	Single-Atom Catalysts (SACs)	Maximum atom utilization, selective activity
	NiFe Layered Double Hydroxides (LDHs)	Efficient oxygen evolution catalysts
	Bismuth Vanadate (BiVO ₄)	Visible-light photoanode
	Doped TiO ₂ Nanostructures	Visible-light responsive photocatalyst
	BaZr _{0.8} Y _{0.2} O _{3-δ} Ceramics	Proton-conducting oxide
	SnSe (Tin Selenide)	Record thermoelectric efficiency (ZT > 2.6)
	Half-Heusler Alloys (TiNiSn, etc.)	High-temperature stability
	Skutterudites (CoSb ₃ -based)	Improved via nanostructuring
Electronic Materials	Graphene	2D carbon sheet, ultrahigh mobility
	MoS ₂ and other TMDs	Semiconducting 2D materials
	Black Phosphorus (Phosphorene)	Direct bandgap, anisotropic transport
	h-BN (Hexagonal Boron Nitride)	2D insulator, smooth substrate
	Topological Insulators (Bi ₂ Se ₃ , Bi ₂ Te ₃)	Conducting surface states
	Organic Semiconductors (P3HT, TIPS-Pentacene)	Solution-processable, flexible
	Perovskite Semiconductors	Tunable bandgap, low-cost synthesis
	Weyl/Dirac Semimetals (TaAs, Cd ₃ As ₂)	Exotic electronic states

	Diluted Magnetic Semiconductors (GaMnAs)	Spin-polarized transport
	MXenes	Metallic conductivity, flexible
	Conductive Polymers (PEDOT:PSS)	Stretchable and transparent

Conclusions

The trajectory of advanced materials from the 19th to the 21st century is proof to the increasing sophistication of human engineering. Each century built upon the last, solving the dominant problems of its time: mass structure, information technology, and now, sustainable, intelligent functionality. The coming era of materials science will be shaped by a synergistic blend of computation, chemistry, and physics, enabling the creation of materials that transform our world. The primary objective of materials research is to derive exceptional properties from substances through rational design and control modification, thereby enabling the development of next-generation technologies. In the 21st century, the field of materials science progressed at an unprecedented pace, marked by the discovery of novel materials exhibiting extraordinary physical, chemical, and electronic properties that surpass those of conventional systems. Current research efforts are predominantly directed toward applications in energy storage, energy conversion, quantum computing, and advanced electronic devices.

During the first quarter of this century, several emerging materials have demonstrated the potential to serve as viable alternatives to traditional materials, laying the foundation for transformative technological advancements. The remaining decades are expected to witness extensive integration of these materials into practical devices, significantly influencing multiple technological sectors. Consequently, the future of materials science holds immense promise, with forthcoming generations anticipated to benefit from and routinely utilize devices derived from these advanced materials.

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Author (s)



Dr. Ravi Kashikar

Department of Basic Sciences, Institute of Infrastructure,
Technology, Research and Management (IITRAM),
Ahmedabad, Gujarat



Dr. Vidyashree Hebbar