

# 33 Unresolved Questions in Nanoscience and Nanotechnology

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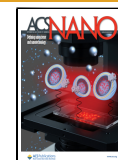
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**ABSTRACT:** Significant advances in science and engineering often emerge at the intersections of disciplines. Nanoscience and nanotechnology are inherently interdisciplinary, uniting researchers from chemistry, physics, biology, medicine, materials science, and engineering. This convergence has fostered novel ways of thinking and enabled the development of materials, tools, and technologies that have transformed both basic and applied research, as well as how we address critical societal challenges. In this Nano Focus, we pose and explore 33 questions whose answers could profoundly impact fields such as energy, electronics, the environment, optics, and medicine. These questions highlight the need for deeper foundational understanding, improved tools and techniques, and innovative applications—each with significant societal relevance. Together, they represent a global call-to-action for the scientific community.



Nanoscience and nanotechnology have perhaps done more than many other modern disciplines to unite researchers across chemistry, physics, materials science, biology, engineering, and medicine (Figure 1). Originally pioneered by physicists, the field saw early

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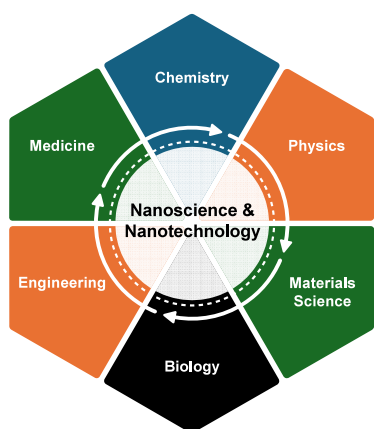


Figure 1. Nanoscience and nanotechnology have united disciplines.

breakthroughs in preparing and characterizing materials at the nanoscale—for instance, the 1986 Nobel Prize in Physics recognized the invention of the scanning tunneling microscope and the electron microscope.<sup>1</sup>

By the 1990s, chemists joined the field in large numbers. The 1996 Nobel Prize in Chemistry, awarded for the discovery of fullerenes,<sup>2</sup> transformed our understanding of carbon, arguably the most important element in the Periodic Table, and sparked further discoveries such as of carbon nanotubes and graphene. This transdisciplinary approach established a model for innovation that fields like synthetic biology and artificial intelligence (AI) are now emulating. Today, nanoscience and nanotechnology tools are integral to disciplines ranging from chemistry to engineering and medicine, continuing to drive scientific, technological, and societal (e.g., policy, education, intellectual property) advancement; these fields have also been important in connecting the scientific community to the lay public.

Looking forward, nanoscience and nanotechnology are well-positioned to address critical global challenges. In this Nano Focus, we present 33 questions—each accompanied by an answer—designed to foster cross-disciplinary dialogue and collaboration. The number of questions corresponds to the number of years of the existence of one of our laboratories (C. A. M.) at the time this project was initiated, a hub of extensive and collaborative research efforts, and also closely coincides with the number of years since many foundational papers in nanoscience and technology appeared in print. The Mirkin lab at Northwestern University (NU) was established in 1991, and NU also hosts the International Institute for Nanotechnology (IIN), founded in 2000, which has grown into one of the world's largest centers for nanoscience research and education. This dynamic research and training environment has significantly contributed to the sustained growth of the field, having contributed to the education of hundreds of faculty members now leading research programs at top institutions worldwide, including many authors of this Nano Focus.

We have organized the 33 questions and responses according to the framework proposed by the Chemical Abstracts Service (CAS) of the American Chemical Society (ACS),<sup>3</sup> which classifies Nobel Prize-recognized innovation into three categories: (1) Foundational Understanding (11 questions), (2) Tools and Techniques (7 questions), and (3) Impactful Applications (11 questions) (Figure 2). Additionally, we explore four questions related to the societal implications of

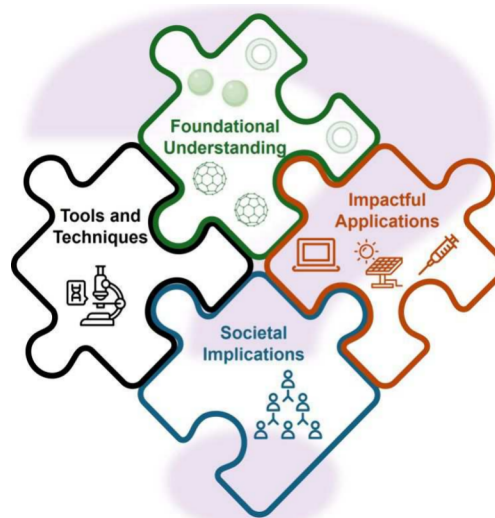


Figure 2. Key unresolved questions in nanoscience and nanotechnology encompass: Foundational Understanding, Tools and Techniques, Impactful Applications, and Societal Implications.

nanotechnology. Addressing the challenges outlined in this article would lead to transformative scientific and societal progress. We offer this Nano Focus as a call-to-action—urging researchers across disciplines to come together in pursuit of integrated, collaborative solutions to some of the most complex problems of our time.

## FOUNDATIONAL UNDERSTANDING

According to the CAS,<sup>3</sup> foundational understanding refers to insights from basic research that deepen our knowledge of the world. In nanoscience and nanotechnology, this targeted insight involves exploring how materials can be designed and synthesized to achieve programmable properties beyond those found in nature. Researchers aim to understand the behavior of these novel materials in complex environments. A key area of interest is reverse engineering: starting with desired properties, identifying suitable materials, and synthesizing them through chemical or top-down physical methods. An ultimate goal is to develop design principles by integrating theoretical models with experimental data. Such concepts form the basis of the discussions in this section.

## DESIGNING AND SYNTHESIZING NEW FORMS OF MATTER WITH CHEMICAL PRECISION

**1. When is atomic and molecular precision in nanostructure synthesis most important, and how can it be achieved?** Atomic and molecular precision in nanostructure synthesis is essential when specific material properties, such as electronic, catalytic, or optical behavior, depend on well-defined structure–property relationships. This level of control is particularly important for fundamental studies aimed at understanding how nanomaterials behave under different conditions and in applications that require reproducible and high-performance materials.

Significant advances have been made. Individual atoms can be positioned on surfaces.<sup>4–6</sup> Hundreds of routes to atomically precise metal nanoclusters (e.g., Au<sub>25</sub>(SR)<sub>18</sub> via size-focusing methods) and reactions involving them exist.<sup>7–9</sup> Dendrimer-templated approaches enable particle uniformity without the intentional use of surface ligands.<sup>10</sup> The hot-injection method

has become foundational in synthesizing well-defined nanocrystals (2–100 nm), while ligand-assisted and electrochemical strategies provide further control over morphology and exposed facets.<sup>11–16</sup> Bimetallic nanostructures can also be engineered to localize specific elements, tailoring surface activity for catalysis.<sup>17–19</sup> These synthetic innovations have enabled hierarchical assemblies with emergent properties.<sup>20–23</sup> The degree of precision required depends on the application. In catalysis, parameters like oxidation state, surface facets, (crystal) phases, and adsorbates significantly affect activity.<sup>15,19,24–28</sup> In optics and electronics, defect structures modulate performance-critical properties such as photoluminescence and conductivity.

Despite these developments, much of the field still relies on empirical optimization. To transition toward predictive synthesis, researchers must develop a mechanistic understanding of nanostructure growth, refine thermodynamic and kinetic control, and identify critical parameters for each application. In catalysis, where active sites may form dynamically under reaction conditions, *in situ* tools capable of resolving atomic transformations are essential.<sup>10</sup> Current ensemble methods like X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS) must be complemented by single-particle and correlative techniques,<sup>29</sup> and theoretical tools such as density functional theory (DFT) and electromagnetic modeling remain invaluable. Emerging integration of machine learning (ML) and AI<sup>30,31</sup> offers new potential to map synthesis conditions to desired outcomes, setting the stage for the routine and automated creation and scale-up of atomically precise nanostructures.

**2. What innovations are needed to make nanomaterials functional in extreme environments?** Nanomaterials designed for use in extreme environments, such as high temperature, pressure, mechanical strain, or radiation or high or low pH, must maintain stability and performance despite their inherently high surface reactivity. While their tunable properties offer opportunities for enhanced performance (e.g., improved catalytic activity under high pressure), these same traits can lead to structural degradation under harsh conditions.<sup>32,33</sup>

A critical need is for *operando* and *in situ* characterization techniques that track atomic-scale structural changes in real time. Tools like electron microscopy and X-ray spectroscopies have begun to simulate extreme conditions, but more robust methods with high spatiotemporal resolution are needed to inform stability design.<sup>34–36</sup> Theory has been used to develop optical control methods based on the phase, intensity, or spectral composition of light. Although researchers have applied such methods to control, and in some cases to understand, complex systems, including molecular-scale electronics, some are not practically feasible or experimentally implementable in the laboratory. In that respect, moderately intense, short-pulse laser fields have an advantage.<sup>37</sup> Computational approaches like DFT and molecular dynamics offer valuable insight<sup>38–40</sup> but often fall short due to assumptions that simplify environmental complexity.<sup>41</sup> Improved algorithms and integration with AI can better capture real-world conditions and expand predictive power across broader chemical spaces.

Materials innovations are also essential. High-entropy alloys (HEAs), composed of multiple metals with near-equimolar ratios, offer exceptional thermal and mechanical stability due to entropy-driven phase stabilization and sluggish diffusion.<sup>42–44</sup>

Ceramics and ceramic matrix composites, including those composed of borides, nitrides, and carbides, exhibit extreme hardness and thermal resistance,<sup>45,46</sup> making them suitable for aerospace and nuclear applications. Two-dimensional (2D) materials like graphene and MoS<sub>2</sub> also show promise due to their flexibility, chemical inertness, and thermal conductivity.<sup>47</sup> Even promising materials can fail in deployment without consistent production routes. Interdisciplinary progress, merging advanced synthesis, ML-guided simulation, and real-time characterization, is key to designing nanomaterials that are not only functional but also reliable in environments far from equilibrium.

**3. Given the rise of structural nanomedicine, how can we design nanomedicines with molecular precision for optimized therapeutic potency?** Molecularly precise nanomedicines represent a new frontier in therapeutic design, offering control over drug identity, spatial arrangement, and hence physicochemical properties. Unlike conventional formulations or larger self-assembled structures, structural nanomedicines,<sup>48–51</sup> by controlling structural presentation in addition to composition, allow fine-tuning of performance metrics—such as circulation time, cellular uptake, and therapeutic potency—while minimizing toxicity.<sup>52–62</sup>

Uniformity is key. Precision synthesis ensures batch-to-batch reproducibility,<sup>53,55,63–66</sup> enabling clearer interpretation of pharmacokinetics and biological interactions. Extended circulation, often achieved through poly(ethylene glycol) (PEG)-ylation, improves bioavailability and therapeutic index.<sup>67,68</sup> Targeting is enhanced through surface modification, such as antibody conjugation<sup>69–79</sup> or physical tuning of size, charge, and shape, to navigate biological barriers like the blood–brain barrier (BBB).<sup>80–82</sup> Methods are needed to formulate nanoparticles as well as to measure the density and positioning of various ligands on nanoparticle surfaces, which is not always straightforward using current methodologies.

Controlled-release systems responsive to pH, enzymes, or metabolic cues enable site-specific activation, increasing efficacy while limiting systemic exposure.<sup>83–88</sup> Paracrine-transfer mechanisms, where particles enter one cell and are passed to neighbors, can also enable staged delivery for localized and sustained treatment.<sup>89</sup> Exploring broader size ranges expands application potential; smaller nanomaterials (3–10 nm) enter cells more efficiently, can engage key biological targets more selectively, penetrate tissues more deeply, and help avoid immune clearance.<sup>90–93</sup> Larger mimetic structures (300 nm–1  $\mu$ m), such as red blood cell-mimicking carriers or membrane-coated particles, evade phagocytosis and prolong circulation.<sup>94–99</sup>

Next-generation structural nanomedicines will combine multiple functional agents—e.g., peptides, nucleic acids, proteins, and polymers—to perform synergistic tasks.<sup>92,93,100–104</sup> These multicomponent systems may enable programmable responses, self-amplifying signals, or feedback-controlled delivery. Progress requires advances in *in vivo* analytics, manufacturing, and regulatory frameworks. Only with molecular-level design, standardized production, and real-time tracking will the field of structural nanomedicine fully transform therapeutic paradigms.

## DELINEATING STRUCTURE–FUNCTION RELATIONSHIPS

**4. How can understanding structure–function relationships in natural systems guide the design of**

**synthetic materials with enhanced functionality?** To design synthetic materials that match or exceed nature's capabilities, we must first understand how biological systems use structure to control function. Natural materials like enzymes achieve near-perfect catalytic efficiencies, performing complex reactions with minimal energy loss. These biological exemplars inspire the rational design of nanostructures for applications in catalysis, energy storage, and biomedicine.

A central challenge lies in replicating dynamic, hierarchical, and adaptive functions observed in biology. Unlike rigid synthetic systems, biological structures respond to stimuli and self-regulate, offering pathways toward intelligent, self-assembling materials. Advances in structural biology, including tools that predict protein 3D structures from amino acid sequences,<sup>105</sup> are now being extended to biomolecule–nanomaterial systems using unified structural descriptors.<sup>106,107</sup> These approaches enable predictive control over nanomaterial assembly and reactivity, moving us closer to synthetic analogs of protein machines.<sup>108</sup>

Synthetic mimicry also involves replicating biological interfaces.<sup>109–118</sup> For example, hydrated silicon dioxide mimics the protective effects of water on membranes. Unlike conventional cryopreservation, nanosilicification preserves cells and tissues at ambient temperatures, protecting them from oxidation and UV degradation. Upon rehydration, the silica shell dissolves, and biological function is restored, offering a cost-effective solution for storing sensitive biological samples.

Another emerging frontier is phase-separated nanomaterials inspired by cellular compartmentalization *via* liquid–liquid phase separation. These transiently ordered systems do not rely on static structure but instead gain function through reversible organization. Such materials challenge the classical “structure defines function” paradigm, providing a foundation for adaptive nanotechnologies.

Ultimately, by learning how living matter controls function through structure, motion, and environment, researchers can engineer synthetic systems that not only mimic biology but extend it, offering new tools for sustainable energy, responsive medicine, and materials with life-like properties.<sup>119,120</sup>

**5. How can structure–function relationships be leveraged to control charge dynamics in nanoscale systems?** Understanding and exploiting structure–function relationships is key to manipulating electronic charge at the nanoscale.<sup>121</sup> Charge dynamics, encompassing generation, separation, motion, and recombination, govern many quantum phenomena and device functionalities. Carefully engineered materials, such as type-II heterojunctions, exploit band offsets to separate electrons and holes spatially after photoexcitation.<sup>122</sup> For example, lead-halide perovskite/metal oxide heterostructures facilitate directional charge transfer, enhancing photocatalytic and photovoltaic performance.<sup>123–128</sup> Materials discovery in this area is critical.

In addition, capturing these ultrafast events, which occur on femto- to attosecond time scales and nanometer length scales, requires advanced characterization.<sup>129–133</sup> Transient absorbance (TA) spectroscopy and nonlinear optical methods, such as second harmonic generation (SHG), provide femtosecond resolution and are sensitive to electric fields and excited-state dynamics. Pushing these technologies to higher spatiotemporal resolution remains critical for real-time insights into charge behavior.<sup>134</sup> Theory also has been a major tool in the development of ultrafast, space-resolved control and analysis

of electronic behaviors. Numerically, it is straightforward to predict and to analyze electronic behaviors down to the ultimate time- and space-resolved limits because wavepacket propagation methods are improving with the efficiency of Fourier transform techniques. Additionally, semiclassical methods, which are typically useful for multidimensional systems and for describing molecules coupled to an environment, quickly become efficient.

Scanning probe techniques and high-resolution electron microscopy complement optical methods by revealing the nanoscale landscape over which charges move. Atomic-resolution imaging of charge domains, defects, and interfaces helps correlate structure with electronic function.<sup>135–141</sup> Enhancing *in situ* electron microscopy and enabling *operando* imaging of devices can convert these tools into “nanolabs” where electronic and structural evolution can be tracked simultaneously.<sup>142</sup>

Emerging tools like ultrafast electron microscopy (UEM) combine the time resolution of spectroscopy with the spatial resolution of electron imaging.<sup>143–145</sup> Similarly, electron holography can quantify electrostatic potentials at atomic resolution and assess single-particle charge states,<sup>146,147</sup> and time-resolved scanning tunneling microscopy, often based on plasmonics, is also important.

Together, these complementary techniques will advance our understanding of charge manipulation, enabling the precise design of nanomaterials for quantum computing, neuromorphic systems, and high-efficiency energy devices. As structure increasingly dictates electronic behavior at the nanoscale, structure–function insights will be vital to developing materials that exploit quantum phenomena with high fidelity.

## SCALING AND INTEGRATING NANOMATERIALS INTO FUNCTIONAL SYSTEMS

**6. How can nanomaterials be scaled and integrated into larger structures and functional devices?** Once a nanomaterial with promising properties has been developed, the challenge shifts to producing it at scale and integrating it into macroscale systems. Many existing synthesis techniques, such as high-throughput nanolithographies and microfluidics, enable the creation of complex nanostructures with useful catalytic, optical, or electronic functions.<sup>148–161</sup> However, translating some of these types of methods to production at industrially relevant scales remains a significant hurdle.

A core issue is the inherently dilute nature of nanoparticle suspensions.<sup>162</sup> Producing dense solids from dilute systems requires large volumes of solvent, making the process inefficient. To overcome this challenge, researchers are developing methods that allow stable, high-concentration nanoparticle solutions while retaining control over interparticle interactions for a variety of applications, including optics.<sup>163</sup> Ligand design is critical because ligands not only stabilize particles but also govern assembly, interfacial behavior, and functional properties.<sup>164–179</sup> Building comprehensive, scalable ligand libraries, including DNA, small molecules, and synthetic polymers, is essential. Researchers in related fields have also sought to solve similar issues to increase the chemical content of metal and ceramic inks of various compositions for use in patterning and additive manufacturing.<sup>180,181</sup>

Processing nanoparticles into bulk materials or functional devices poses additional challenges.<sup>155,182</sup> While superlattices formed from nanoparticles can mimic atomic crystals, their

growth dynamics differ markedly due to the larger sizes and weaker forces at play.<sup>183,184</sup> The kinetics of these processes affect material microstructure.<sup>185–190</sup> While atomic solids rely on microstructural control for property management, their effects on nanoparticle assemblies remain less explored. New assembly methods must account for these mesoscale phenomena, enabling precise delivery of thermal, mechanical, or electromagnetic energy during fabrication.

Integration into devices requires maintaining nanoscale functionality within macroscale architectures. This integration might involve embedding nanoparticles in flexible substrates, 3D printing nanocomposites, or creating multiscale heterostructures. As materials are scaled, interfaces become crucial, dictating performance and failure modes. Future progress depends on understanding the multiscale thermodynamics, kinetics, and mechanics of nanostructure assembly and integration. Bridging the gap between nanoscale precision and macroscale utility will unlock transformative applications in energy systems, computing, healthcare, and structural materials.

**7. How can we integrate nanoscale components and processes with larger-scale systems to create devices with hierarchical structure and function across length and time scales?** Integrating nanoscale components into larger-scale systems to create functional devices with structural and temporal hierarchies remains a central challenge in nanoscience. Biological systems provide compelling models, where nanoscale machineries exhibit highly organized architectures and operate synergistically across spatial and temporal dimensions.<sup>191,192</sup> Mimicking such multiscale coordination in engineered systems requires precise definition of nanoscale building blocks and seamless connection across length scales.<sup>193</sup>

Top-down fabrication methods, such as wafer-scale photolithography, offer high spatial precision but face limitations in scalability and cost.<sup>194</sup> Bottom-up strategies, including the synthesis and self-assembly of nanoparticles and nanoclusters, enable complex organization from the molecular level upward.<sup>195</sup> A hybrid approach combining these methods is critical for constructing hierarchical structures with tailored geometries and functions.

Recent work has demonstrated controlled assembly of nanoclusters into superstructures for optical and electronic applications,<sup>182,196–201</sup> yet achieving arbitrary geometries with robust integration remains difficult. Advances in ML are addressing this gap by enabling predictive design across scales.<sup>202</sup> Inspired by protein folding breakthroughs like AlphaFold,<sup>203,204</sup> ML models now predict properties of atomic clusters,<sup>205,206</sup> metal–organic frameworks (MOFs),<sup>207,208</sup> and perovskites,<sup>209,210</sup> helping bridge nanoscale traits with macroscopic material performance (see also Question 9 below).

Temporal hierarchies are vital. Many critical nanoscale processes, such as electrocatalysis, occur over femtosecond to second time scales.<sup>211,212</sup> Designing devices that leverage these processes requires synchronizing kinetic and structural hierarchies.<sup>213</sup> This strategy motivates the development of responsive, multilength-scale architectures optimized for dynamic function.

Progress depends on advanced characterization. *In situ* and *operando* microscopies,<sup>214</sup> correlative techniques,<sup>215</sup> and ultrafast spectroscopies<sup>216</sup> enable simultaneous monitoring of structural and functional dynamics, providing key insights into multiscale interactions. These tools and strategies drive

the rational design of integrated devices that exploit nanoscale phenomena for macroscopic utility.

**8. How can nanoenabled devices be seamlessly integrated with biological systems to improve human health?** Seamless integration of nanoenabled devices with biological systems holds great promise for transforming healthcare, but it requires careful attention to both materials and systems design. Recent advances in wearable and implantable nanodevices have demonstrated exciting capabilities for diagnostics, monitoring, and therapy.<sup>217–222</sup> However, true integration demands that devices operate harmoniously within the complex and dynamic human body as has been accomplished in certain cases with larger scale systems (e.g., implantable defibrillators with batteries that last approximately 10 years and are Bluetooth-enabled and capable of communicating data to hospitals *via* an app).

Materials in direct contact with biological tissue must be biocompatible, avoiding immune responses or fibrosis, and resilient to mechanical strain over time.<sup>223–225</sup> Mismatches in mechanical properties between soft tissues and rigid electronics can cause damage and limit long-term stability. To address this issue, researchers are developing shape-adaptive interfaces that match the mechanical compliance of tissues, improving integration and minimizing inflammation.<sup>226–229</sup>

For skin-mounted devices, breathability is critical to ensure user comfort and prevent irritation. Natural materials such as silk have emerged as promising substrates due to their biocompatibility, flexibility, and gas permeability.<sup>230–234</sup> These innovations are key to developing unobtrusive, long-term health monitors.

Powering such miniaturized systems remains a major hurdle. Conventional batteries are bulky, rigid, and often require invasive replacement procedures.<sup>235</sup> Bioenergy harvesters, which convert mechanical, thermal, or biochemical energy from the body into usable electricity, represent a compelling alternative and are under active development.<sup>236,237</sup> On the system level, high-resolution nanosensors generate large volumes of real-time data, necessitating robust data management and wireless communication platforms.<sup>238</sup> Ensuring data security, processing speed, and scalability will be essential for widespread clinical use.

Ultimately, nanoenabled devices must evolve into “smart” systems that sense biological signals and autonomously respond to disease states. Integrating AI enables these devices to analyze complex data sets, personalize treatment, and enhance early detection.<sup>239,240</sup> These advances are reshaping how we interface electronics with the human body, paving the way for the next generation of personalized, responsive healthcare technologies.

## MULTISCALE MODELING OF NANOMATERIALS

**9. How can we model materials across length scales where classical or quantum mechanics alone are inadequate to match theory and experiment?** Modeling materials across multiple scales—from atoms to devices—is crucial for understanding complex nanomaterial behavior, yet no single theoretical framework suffices across all regimes. Classical and quantum mechanics each provide foundational insights: quantum mechanics excels at capturing electronic properties of small systems, while classical molecular dynamics (MD) and Monte Carlo methods model larger systems using empirical or quantum-derived forces.<sup>241</sup> However, these

methods face limitations in scale, accuracy, or computational cost.<sup>242</sup>

For very large systems or long time scales, coarse-grained models group atoms into simplified units, or “beads,” enabling simulations of polymers, DNA, proteins, and nanoparticle superlattices.<sup>243–251</sup> Yet, such models struggle with chemical processes like bond formation or redox reactions, especially at interfaces between dissimilar materials. At coarser levels, continuum theories are applied, but often lack the resolution needed to capture mesoscale phenomena and may be constrained by computational resources.<sup>252–254</sup>

To bridge these gaps, multiscale modeling approaches have emerged. Hybrid schemes, such as mixed quantum-classical or semiclassical models, are particularly effective for describing light-matter interactions. For example, finite-difference time-domain (FDTD) and finite element methods (FEM) are widely used in classical electrodynamics,<sup>255,256</sup> while quantum electrodynamics is necessary to understand nanoscale optical phenomena such as in quantum dots, plasmonics, and strong light-matter coupling.<sup>257,258</sup> Mixed and semiclassical methods provide a balance between computational efficiency and quantum accuracy.<sup>259–262</sup>

Both ML and AI are increasingly integrated into multiscale frameworks to accelerate simulations, improve force field accuracy, and model complex phenomena. Notable successes include protein folding predictions<sup>203</sup> and ML-derived interatomic potentials,<sup>263</sup> as well as reaction modeling.<sup>264</sup> These data-driven approaches can complement physics-based methods, particularly in challenging intermediate regimes where neither classical nor quantum mechanics alone are sufficient. Ultimately, combining coarse-graining, hybrid quantum-classical methods, and ML offers a path to unify theoretical and experimental understanding across scales, essential for the predictive design of next-generation nanomaterials.

## UNDERSTANDING AND EXPLOITING NANOMATERIAL LIFECYCLES

**10. Given that nanostructures are often dynamic under external stimuli, how can we predictably control nanoparticle durability—and can self-healing mechanisms be designed to prolong functionality?** Nanostructures are inherently dynamic, responding to stimuli such as light, heat, and electrochemical input in ways that can both enhance functionality and accelerate degradation.<sup>265,266</sup> While this dynamism enables tunable behavior, it introduces challenges for their long-term durability, particularly in high-performance applications like energy storage, catalysis, and sensing. Designing nanoparticles that respond to repeated stimulation in a predictable and robust manner is therefore critical.

One promising strategy is to draw inspiration from biological systems, where self-repair is common. Adaptive nanostructures capable of reconfiguring or restoring their function after damage could maintain performance over extended use.<sup>267</sup> Such self-healing materials might incorporate built-in feedback mechanisms that detect structural failure and initiate repair without significant external input. However, the complexity of these systems makes material selection and integration of self-repair functions particularly challenging.

An equally important design consideration is end-of-life behavior. Rather than maximizing durability indefinitely, in some cases it may be desirable to enable controlled

degradation after functional use. Degradable coatings or modular architectures can facilitate the recovery of valuable components and reduce environmental impact.<sup>268–274</sup> For instance, soft materials like nanocellulose offer built-in degradability,<sup>275</sup> while coordination chemistry has been used to recover gold atoms from nanoparticles using benign agents such as cyclodextrins.<sup>276</sup> These strategies highlight the potential to design nanoparticles not only for performance but also for sustainability and recyclability.

Ultimately, future nanostructures should balance resilience and responsiveness during their operational lifespan with environmentally and economically beneficial disassembly at end-of-life. This dual focus on durability and degradability will be essential for sustainable nanotechnology in advanced applications.

**11. What are the key factors in nanometabolomics, and can we design nanometabolites to act as therapies rather than just byproducts?** Nanometabolomics—the study of how nanomedicines are metabolized—plays a critical role in understanding and optimizing the safety and efficacy of nanoscale therapeutics. The pharmacokinetics (PK) and pharmacodynamics (PD) of nanomedicines depend heavily on size, shape, surface chemistry, and composition,<sup>277–280</sup> yet these parameters remain insufficiently characterized in many systems. Once inside the body, nanoparticles can exhibit complex and unpredictable behavior,<sup>281</sup> necessitating early identification and characterization of resulting nanometabolites.

To ensure safe and effective use, these nanometabolites must be examined not only for toxicity but also for therapeutic potential. This shift—from viewing nanometabolites as waste products to potentially useful agents—could open new avenues for therapy. Accurate ADME (absorption, distribution, metabolism, and excretion) profiling, integrated with physiologically based pharmacokinetic (PBPK) models, is essential for understanding *in vivo* behavior.<sup>282,283</sup> These models are especially useful when guided by ML, enabling prediction of nanomedicine fate from *in vitro* data.

Complexities multiply with multicomponent nanomedicines, where component interactions affect PK/PD in ways not captured by single-entity models.<sup>61,65,284–297</sup> These formulations require advanced, systems-level models that account for structural organization, degradation pathways, and the roles of individual components—including beneficial nanometabolites.

A key complicating factor is the formation of a “protein corona” around nanoparticles upon exposure to biological fluids.<sup>298</sup> This corona modulates interactions with cells and organs, profoundly affecting ADME and immune responses. Protein identification, ideally conducted *in vivo via* mass spectrometry, is vital,<sup>299</sup> though conventional techniques are often incompatible with soft nanomaterials.<sup>300</sup> Moreover, corona composition varies with administration route, patient physiology, and even lab-specific conditions, underscoring the need for standardized analytical protocols.<sup>301,302</sup>

Integrating mass spectrometry data with PBPK models could enable predictive mapping of protein-nanoparticle interactions to biological outcomes. Ultimately, refining nanometabolomics will not only ensure safer nanomedicines but also allow rational engineering of therapeutic nanometabolites, transforming how we design and deploy nanoscale treatments.

## TOOLS AND TECHNIQUES

Tools and techniques encompass innovations that enable new research methods, significantly enhancing or accelerating scientific progress.<sup>3</sup> Nanomaterials, with their unique structures and properties distinct from both molecules and bulk materials, require specialized tools for analysis. Characterization techniques have evolved alongside synthetic methods and have been essential to the field's development. Device fabrication also plays key roles in translating nanomaterials into practical applications. More recently, AI and ML have become integral to nanoscience, offering advanced solutions for data analysis, predictive modeling, and problem solving. Additionally, cross-disciplinary tools are crucial for fostering collaboration and accelerating progress. Universal platforms that operate across various materials and domains would promote greater efficiency, integration, and innovation.

## DEVELOPING NEW SYNTHETIC PROTOCOLS WITH SUSTAINABILITY IN MIND

**12. How can we design nanomaterial syntheses to be sustainable across raw materials, reactions, and manufacturing processes?** To minimize the environmental and human health impact of nanotechnology tools, nanomaterial syntheses must embrace sustainable principles from the outset. This includes using renewable feedstocks, environmentally benign reagents, and energy-efficient methods. Green synthesis pathways should prioritize atom economy, favoring reactions that maximize the incorporation of raw materials into the final product, while minimizing waste and side products.<sup>303–306</sup> Lifecycle analyses should be routinely applied to evaluate environmental costs from synthesis through disposal and paired with standardized sustainability guidelines.<sup>307</sup> Predictive tools, such as ML, can assist by modeling the environmental and biological impacts of nanomaterials, accelerating the discovery of safer and more sustainable alternatives.<sup>308</sup>

Biomass-based nanomaterials—derived from abundant, biocompatible feedstocks—are particularly promising.<sup>309–314</sup> For example, cellulose-based materials have been employed in solar steam generation,<sup>315</sup> lignin-derived hydrogels in drug delivery,<sup>316</sup> plant polyphenols in nanolithography,<sup>317</sup> and protein templates in the synthesis of metal nanoparticles, quantum dots, and polymers.<sup>318–321</sup> Environmentally friendly reaction conditions, such as ambient temperature, aqueous solvents, microwave or ultrasound-assisted reactions, and enzyme catalysis, should continue to be explored.<sup>322–325</sup>

Advances in automation and high-throughput synthesis can further reduce energy consumption and increase reproducibility.<sup>326–329</sup> However, sustainability challenges remain, particularly with biomolecules like DNA that are frequently used in nanomaterial assembly.<sup>71,330,331</sup> Traditional phosphoramidite-based DNA synthesis involves toxic solvents and excessive reagents.<sup>332</sup> Alternatives such as enzymatic synthesis with terminal deoxynucleotidyl transferase (TdT),<sup>333–336</sup> improved solid-phase techniques,<sup>337–339</sup> and P(V)-based coupling reagents<sup>340–342</sup> are emerging. Sustainable syntheses of modified nucleic acids like deoxynucleic guanidines have been achieved using iodine in place of mercuric chloride.<sup>343,344</sup>

Ultimately, sustainability should be integrated into every stage of nanomaterial development—from molecular design and reaction conditions to manufacturing scale-up and end-of-life disposal. Making sustainable nanomaterial synthesis the

default rather than the exception will require both technological innovation and cultural shifts within the research community.

## DEVELOPING NEW TOOLS TO STUDY THE NANOSCALE WORLD

**13. What tools are needed to study single nanomaterials and assemblies in native, dynamic environments?** Conventional characterization techniques often average the properties of nanomaterials over space and time, obscuring critical insights into dynamic behavior at the single-particle level.<sup>345</sup> To understand nanoscale processes as they occur in real-world environments, new tools must deliver high-resolution, temporally resolved data *in situ* and *operando*.

Radiation-based approaches (e.g., electron, ion, or photon probes) and scanning techniques like scanning probe microscopy (SPM) provide localized information.<sup>346</sup> Advanced transmission electron microscopy (TEM) now enables atomic-scale resolution, 3D tomography, and real-time studies of materials under environmental stimuli.<sup>347–351</sup> To realize these capabilities, multimodal platforms that integrate nanofabricated specimen stages with imaging, spectroscopy, and data analyses are needed.<sup>352,353</sup>

Instrumentation must continue to evolve: coherent sources, aberration correctors, high-dynamic range detectors, and encapsulated micro/nanofabricated chips allow imaging under realistic temperature, pressure, liquid, or gas conditions.<sup>354</sup> Innovations like *in situ* TEM stages with microfluidics and environmental controls enable direct observation of structural evolution.<sup>355</sup> Stimuli such as light, force, or X-rays can be applied within these systems to explore nanoscale responses. Both AI and ML are critical enablers of next-generation analysis. Integrated into tools like 4D STEM or atomic force microscopy (AFM), they enhance acquisition speed, automate processing, and improve reproducibility.<sup>356,357</sup> ML models trained on large data sets can detect trends, direct attention to emerging events in real time, and even adapt experimental parameters on-the-fly.

Ultimately, researchers must develop a new generation of instruments that combine minimal sample impact with high-throughput, high-precision analysis of nanoscale behavior. These tools will provide insight into how nanomaterials evolve, interact, and function—unlocking a deeper understanding of their mechanisms and informing better design across applications.

**14. How can nanotechnology be used to build engineered tissues and organs for biological research and medicine?** Nanomaterials offer powerful capabilities to replicate biological complexity in engineered systems.<sup>358</sup> By mimicking the nanoscale structure of extracellular matrices (ECMs), materials such as electrospun fibers, hydrogels, and nanoparticles can support cellular adhesion, growth, and differentiation.<sup>359–362</sup> These scaffolds can be engineered to deliver spatially and temporally resolved chemical and mechanical signals, enabling detailed study of biological processes and disease states.<sup>363–369</sup>

Advances in 3D printing using nanocomposite inks now enable fabrication of vascularized organ-like structures.<sup>370</sup> Integration of nanomaterials into these systems permits embedded sensing of stress, pH, or metabolite levels over time.<sup>371–373</sup> These capabilities are being used to explore phenomena such as metastasis in flowing environments,<sup>374</sup>

stem cell differentiation through electrical signals,<sup>375</sup> and protein expression in response to drugs or toxins.<sup>376</sup>

Organ-on-chip (OoC) models have gained attention for their ability to recreate organ-specific microenvironments.<sup>377,378</sup> During the COVID-19 pandemic, they accelerated drug testing. The emerging field of body-on-chip (BoC) platforms connects multiple OoCs to simulate systemic human physiology.<sup>379,380</sup> These platforms offer new possibilities for personalized medicine and miniaturized clinical trials.<sup>381</sup>

Real-time monitoring remains a key challenge. Nanobiosensors, including electrochemical, mechanical, and optical devices, can detect biomarkers such as troponin in cardiac chips, glutamate in brain models, or oxygen in tumor environments.<sup>382–385</sup> Cyborg organoids, living tissues integrated with stretchable nanoelectronics, enable continuous sensing of cellular activity, a significant advance in studying tissue responses.<sup>386,387</sup>

To scale these systems and to ensure reproducibility, interdisciplinary efforts are needed. Biologists and engineers must codesign platforms that balance biological relevance with manufacturability and analytical access. With ongoing improvements in nanomaterials and sensing technologies, engineered tissues and organs are becoming indispensable tools for biomedical discovery and therapeutic development.

## MAKING SCIENTIFIC LABOR AND DECISION-MAKING PROCESSES MORE EFFICIENT

**15. How can AI and ML accelerate nanomaterial discovery through inverse design?** Inverse design, identifying a desired property and working backward to find a structure that achieves it, is transforming nanomaterials discovery. AI and ML play pivotal roles in this process by mapping synthesis-structure-property relationships and predicting candidate materials with desired functions.<sup>31,388,389</sup>

Generative ML models such as variational autoencoders and generative adversarial networks can propose new molecular structures with targeted properties.<sup>390,391</sup> However, to ensure trust and transparency, interpretable ML methods, like SHAP (SHapley Additive exPlanations) or physics-informed neural networks, are needed to identify key features driving performance.<sup>392–395</sup>

A major limitation is data. High-quality, large-scale data sets are essential for training ML models. High-throughput experimental methods, megalibraries, and first-principles simulations such as density functional theory (DFT) are generating foundational data, but broader efforts are needed to scale and standardize these processes.<sup>156,159–161,396–400</sup> Public databases like the Open Quantum Materials Database and Materials Project can accelerate access and collaboration.<sup>401–403</sup> Crucially, inverse design requires iterative, closed-loop systems where AI predictions are validated by experiments, which then provide feedback to improve the model. Such loops reduce time and resource use while enabling optimization of materials for specific applications.<sup>404–406</sup>

As the field matures, the combination of AI/ML with automated synthesis, advanced characterization, and open data will transform materials development—from trial-and-error discovery to hypothesis-driven innovation. In nanoscience, where the combinatorial space is immense and structure-property relationships are complex, inverse design offers a powerful path to accelerate the development of next-generation materials. Another type of iterative closed-loop approach, genetic algorithms, has been successfully applied<sup>407</sup>

to design nanoplasmonic devices and invert experimental data into structural information. Because of the stochastic nature of this approach, it is numerically expensive. On the other hand, it has the advantages of stability and generality.

**16. How can AI and robotics be combined to automate laboratory workflows in nanoscience and nanotechnology?** The rapid advances in AI, ML, and deep learning over the past decade are transforming laboratory automation in nanoscience and nanotechnology. Models like convolutional neural networks (CNNs) excel at computer vision tasks, such as vehicle detection,<sup>408,409</sup> while recurrent neural networks (RNNs) and generative pretrained transformer (GPT) models power language understanding and generative tasks.<sup>410,411</sup> Such AI models, combined with robotics, enable automation of routine laboratory tasks, increasing reproducibility and freeing researchers to focus on data analysis and experimental design.<sup>412–414</sup>

The integration of AI and robotics promises scalable, high-throughput experimentation beyond human capacity.<sup>397,415</sup> For example, AI can mine the literature to identify key nanoparticle synthesis parameters. Robotic platforms can then perform, monitor, and characterize syntheses in real time. Iterative feedback using ML models can refine synthesis conditions automatically by correlating parameters to nanoparticle properties. “Self-driving labs” (SDLs) embody this concept, combining robotic automation of repetitive tasks with ML analysis of complex data sets.<sup>397,399</sup> Such SDLs have been used to synthesize nanoparticles, polymers, and organic molecules relevant to pharmaceuticals, catalysis, and clean energy,<sup>416,417</sup> although systems for synthesis under harsh conditions remain limited.<sup>418</sup> Carnegie Mellon University’s Cloud Lab, accessible remotely, is a leading example of such SDL infrastructure.<sup>419</sup>

Successful AI-robotic integration depends on large, high-quality data sets for training.<sup>420</sup> Progress requires building data pipelines, developing interoperable software, and adopting cloud best practices across SDLs. Standardizing data formats, reproducibility protocols, and synthetic description languages would enhance integration among AI, robotics, and characterization techniques.<sup>421,422</sup> Moreover, automated characterization tools—especially for advanced instruments like TEM, SEM, and synchrotron X-ray spectroscopies—should be integrated into SDL workflows.<sup>399,423</sup> Together, these advances point toward fully autonomous laboratories that accelerate discovery and translation in nanoscience and nanotechnology.

**17. How can we improve early stage prediction of nanomedicine efficacy in humans?** Predicting how nanomedicines will perform in humans remains a major challenge that slows development down. Like all drugs, nanomedicines must pass rigorous preclinical testing, including *in vitro* cell culture studies and *in vivo* animal models, before clinical trials.<sup>424</sup> However, these models often fail to predict human outcomes reliably.<sup>425</sup> Cultured human cells are typically transformed immortalized lines or clonal populations that poorly represent patient heterogeneity. Primary human cells are scarce and short-lived. Animal models differ in genetic homology and immune responses, which complicates translation. Many nanomedicines, particularly immune therapies, require intact human microenvironments not replicated in standard models.

Emerging approaches aim to address these limitations. Advanced *in vitro* models, including 3D cultures and microfluidic OoC systems, more closely mimic human tissue

architecture and physiology.<sup>426–432</sup> These platforms are being explored for applications such as tumor vaccine development.<sup>433,434</sup> “Humanized” mouse models, engineered to express human antigens and drug targets, reduce species differences.<sup>435–437</sup> *Ex vivo* manipulation of human tissues from healthy or diseased donors further refines predictive assays.<sup>438</sup> Organoid cultures enable personalized screening, offering the possibility of tailored dosing and treatment strategies.<sup>439–441</sup> Such approaches could improve patient stratification and reduce trial failures by identifying effective therapies earlier.

Computational modeling and AI tools are increasingly employed to predict nanomedicine behavior, incorporating genetic, biomarker, and sex/gender differences.<sup>442–444</sup> Sex-based biological differences remain understudied but can significantly influence immune cell uptake of lipid nanoparticles, for example.<sup>445</sup> Protein corona engineering is being developed to mitigate sex-related immune variability.<sup>446</sup> These multidisciplinary innovations aim to accelerate nanomedicine translation, but more researchers must engage to overcome remaining challenges.

## USING STANDARDIZATION TO DRIVE COLLABORATION

**18. What strategies are advancing standardized, reproducible analyses in nanoscience?** Nanomaterials’ unique properties and the diversity of characterization techniques demand standardized approaches to ensure data reliability, reproducibility, and broad usability.<sup>447,448</sup> Establishing global standards for data acquisition, processing, and interpretation is essential to foster collaboration and to accelerate innovation.<sup>449,450</sup> Large data sets require interoperable frameworks supported by academia, industry, and standardization bodies.

Efforts focus on developing standardized protocols, automated analysis tools, and shared databases. Centralized repositories categorize nanomaterials and their properties, inspired by analogous databases in molecular biology and chemistry (e.g., Protein Data Bank, Cambridge Structural Database). Initiatives include NanoCommons<sup>451</sup> for nanoinformatics safety data, caNanoLab<sup>452,453</sup> and Nanotechnology Characterization Laboratory<sup>454</sup> for nanomedicine safety and characterization, and NaKnowBase (NKB)<sup>455</sup> and Nano-Informatics Knowledge Commons (NIKC)<sup>456</sup> for biological and environmental data. The Materials Project<sup>401,457,458</sup> and Electrolyte Genome<sup>459</sup> gather materials data for energy applications. Nano<sup>460</sup> curates nanomaterial literature data. AI-powered platforms like eNanoMapper<sup>461</sup> automate data analysis to reduce human error and enhance reliability.<sup>462,463</sup>

Standardization also expedites regulatory review and commercialization by providing consistent classifications and reducing redundant testing.<sup>464,465</sup> For example, NIST-developed universal research-grade test materials for SARS-CoV-2 lipid nanoparticles<sup>466</sup> accelerated vaccine development through harmonized analytics and collaboration.<sup>467–469</sup> Similar efforts are expanding to extracellular vesicles and other nanomedicines, highlighting the critical role of standardized clinical efficacy data.<sup>470,471</sup> Continued work is needed to broaden and deepen these standardization frameworks, ultimately hastening safe nanotechnology translation.

## IMPACTFUL APPLICATIONS

Impactful applications refer to technologies that benefit large numbers of people or show strong potential to do so. Like other scientific fields, nanoscience and nanotechnology are driven by curiosity and rooted in fundamental discovery. However, broad scientific impact comes from the ability to translate these discoveries into technologies that improve lives. This translation is a key measure of the value of scientific and engineering advancements. Nanoscience and nanotechnology are already influencing a wide range of applications—from medicine to energy and the environment—reflecting the interdisciplinary nature of the field. These technologies enhance quality of life by enabling better disease treatment and tracking, improving performance, providing clean water and energy solutions, and advancing how we access, analyze, and transmit information.

## ENHANCING INFORMATION PROCESSING, STORAGE, AND SHARING

**19. How can nanotechnology enhance computing and data storage?** Nanotechnology promises to revolutionize computing and data storage by overcoming fundamental limits of silicon-based devices.<sup>472</sup> Innovations at the architecture, materials, and algorithmic levels aim to increase capacity, speed, and energy efficiency critical to meeting growing demands driven by AI and ML.<sup>473</sup>

Nanomaterials such as graphene, quantum dots (QDs), nanosheets, and lanthanide-doped nanocrystals are integral to next-generation memory technologies.<sup>474,475</sup> These materials enable devices like resistive random-access memory (ReRAM) and spintronic memories that are smaller, faster, and consume less power than conventional memories.<sup>476</sup> Quantum computing represents a transformative frontier, utilizing qubits that exploit superposition and entanglement to solve complex problems exponentially faster than classical computers.<sup>474</sup> Nanophotonic circuits, which use photons rather than electrons for data transfer, promise reduced latency and higher bandwidth for future data centers and communication networks.

Biomolecules such as DNA provide another exciting platform for computation and data storage.<sup>472,477,478</sup> DNA’s stability and dense information encoding allow massive parallelism in data processing. Techniques like polymerase chain reaction (PCR)<sup>479</sup> enable efficient data amplification. Recent work explores peptide arrays immobilized on self-assembled monolayers for information storage readable by mass spectrometry, encoding digital data in molecular patterns.<sup>480</sup> These biomolecular approaches open new pathways for ultradense, energy-efficient storage and computing, complementary to traditional silicon and emerging quantum technologies.

**20. How are nanomaterials enabling faster, more secure global communication?** Nanomaterials are key to advancing communication technologies that demand higher speeds, larger capacities, and improved energy efficiencies.<sup>481–483</sup> Two-dimensional (2D) materials such as graphene and other semiconductors exhibit exceptional electrical properties compatible with silicon technologies, enabling nanoscale transistors and photonic devices for rapid signal processing.<sup>484–486</sup> These advances support the development of compact antennas, flexible electronics, and enhanced optical fibers critical to modern networks.<sup>487–490</sup>

Security in global communication increasingly relies on quantum communication, leveraging quantum mechanics to provide theoretically unbreakable encryption. Quantum dots, nanodiamonds, and other nanostructures serve as single-photon emitters and qubit hosts, potentially operable at room temperature, overcoming technical hurdles in quantum information science.<sup>491,492</sup> Integrated photonics and on-chip signal routing reduce energy losses and bolster secure data transfer.<sup>493,494</sup>

These technologies pave the way for reliable, ultrafast, and secure communication networks, addressing the demands of emerging networks for 5G, 6G, and even more advanced communication systems.<sup>495</sup> Nanomaterial-enabled hardware will underpin future communication infrastructure by enhancing bandwidth, reducing latency, and ensuring data integrity on a global scale.

## ENSURING FOOD AND WATER SECURITY

**21. How can nanotechnology improve sustainable agriculture and crop protection?** Nanotechnology offers promising tools to enhance agricultural sustainability, crop yield, and resilience, addressing the United Nations' Sustainable Development Goal 2 of ending hunger and achieving food security.<sup>496</sup> Early research has demonstrated how nanomaterials can improve the delivery efficiency and specificity of pesticides, herbicides, fertilizers, and genetic materials to plants.<sup>497–502</sup> These nanoenabled agrochemicals reduce active ingredient use and environmental runoff while enhancing crop resistance to pests and diseases.<sup>497,503,504</sup>

Nanoformulated fertilizers, such as those based on incongruent dissolution, release essential nutrients more precisely, reducing greenhouse gas emissions and mitigating food insecurity exacerbated by climate change.<sup>505–507</sup> Nanoclays improve water retention and nutrient delivery in arid soils, while carbon and TiO<sub>2</sub> nanoparticles assist in soil remediation by adsorbing pollutants.<sup>508–510</sup> Nanotechnology also improves disease and pathogen detection accuracy in crops and helps protect plants against environmental stresses like drought and nutrient deficiency.<sup>511</sup>

Despite these advances, environmental impacts of nanomaterials on soil microbiota, pH, and plant growth remain underexplored and require further study.<sup>512–514</sup> Insights from the field of nanomedicine, especially lessons in drug delivery, should be leveraged to accelerate the development of safe, effective nanoagrochemicals that bolster agricultural capabilities and performance in diverse environments, including extraterrestrial ones, although techno-economic analyses need to be done.<sup>515,516</sup>

**22. How can nanotechnology be used to ensure global access to clean and safe water?** Global water security depends on increasing access to clean water, including in arid and contaminated regions; indeed, more than two centuries of industrialization has polluted water supplies owing to industrial processes. Porous nanomaterials such as MOFs, covalent organic frameworks (COFs), and hydrogen-bonded organic frameworks (HOFs) have emerged as powerful materials for harvesting water from humid air.<sup>517–520</sup> Their high surface areas and tunable pore chemistries enable selective and efficient water capture.<sup>521</sup> Optimizing hydrophilicity and pore geometry tailors total uptake and working capacity.<sup>522</sup> Integrating MOFs into solar- or heat-driven devices enables passive, energy-efficient water release, advancing decentralized water harvesting technologies.<sup>523</sup>

Nanomaterials also improve desalination and purification processes.<sup>524,525</sup> Carbon nanotube and graphene oxide membranes enhance water transport and salt rejection, while zerovalent iron nanoparticles remove heavy metals.<sup>510,526–528</sup> Rapid 3D printing of filtration resins, like poly(lactic acid)-TiO<sub>2</sub> composites, enables on-demand, decentralized water purification with tailored contaminant capture.<sup>529–532</sup> Moreover, nanomaterials coatings on widely available and cost-effective sponge-based sorbents can be used to clean up contaminated bodies of water.<sup>533–535</sup> Such reusable, multiuse sorbents are selective for the removal of oil/organics, phosphate/fertilizer and metal contaminants. Continued development and implementation of such sustainable approaches are being commercially translated (i.e., Coral Innovations). Future research must focus on scalable, cost-effective synthesis and multicontaminant removal capabilities.

Nanomaterial-based sensors enhance water quality monitoring by detecting contaminants such as heavy metals, organic pollutants, and pathogens at trace levels.<sup>529,536–538</sup> Portable, low-cost devices like colorimetric strips and smartphone readers are under development to improve accessibility.<sup>539–541</sup> Integrating nanosensors with underwater vehicles enables *in situ*, real-time monitoring.<sup>542</sup> These innovations will be critical to ensuring safe drinking water worldwide, supporting environmental and public health.

## SAFEGUARDING THE ENVIRONMENT

**23. How can nanotechnology be applied to identify, sequester, and remediate environmental toxins?** Environmental toxins and pollutants pose serious threats to both human health and ecosystems. Nanotechnology offers innovative solutions by leveraging engineered nanomaterials designed to resist, to capture, and to remediate such harmful substances.<sup>267,543–545</sup> Nanomaterials can be tailored at the surface and structural levels to adjust properties like hydrophobicity, electrostatic charge, pore size, surface area, and active site characteristics, enabling selective microbial resistance,<sup>546,547</sup> targeted pollutant capture,<sup>548</sup> and catalytic toxin transformation.<sup>549</sup> For example, nanoparticles based on earth-abundant metals like aluminum (Al) and copper–iron (Cu–Fe) have proven highly effective in catalyzing the conversion of environmental toxins such as ammonia and hydrogen sulfide.<sup>550–552</sup> Additionally, metal-oxide and carbon nanomaterials and dendrimers are extensively employed in remediation technologies.<sup>553</sup>

MOFs present another powerful approach due to their customizable pores and surface chemistry that facilitate toxin adsorption and degradation.<sup>554–557</sup> Some MOFs incorporate catalytic sites that break down hazardous compounds, including organophosphorus toxins, into less harmful by-products.<sup>556</sup> Such MOFs are used in protective gear against chemical threats.<sup>558</sup> Emerging challenges, such as persistent organic pollutants and microplastics, necessitate next-generation nanomaterials with enhanced selectivity and efficiency.<sup>543</sup> Data-driven materials design and ML platforms accelerate the development of cost-effective, earth-abundant remediation materials.<sup>559,560</sup> Smart adaptive nanomaterials that respond dynamically to environmental stimuli are also being explored.<sup>561</sup>

Nanoparticle-based cross-linking within hybrid materials imparts dynamic, robust, and recyclable properties, enabling extended operational lifetimes and facile separation and reuse.<sup>267</sup> Integrating these nanotechnologies with renewable

energy systems could yield comprehensive pollution management solutions.<sup>548</sup> The convergence of advanced synthesis, characterization, and sustainability drives the development of increasingly effective and environmentally conscious nanomaterial-based remediation strategies.

## SPURRING THE GLOBAL CLEAN ENERGY TRANSITION

**24. How can nanomaterials advance clean energy generation and sustainable fuel production?** Nanomaterials play transformative roles in clean energy generation and the sustainable production of fuels, offering new pathways to reduce reliance on fossil resources.<sup>304–306,562</sup> The global challenge of generating abundant renewable electricity has benefited greatly from nanoscience advancements in solar, wind, hydroelectric, and tidal technologies. For example, photovoltaic (PV) cells have been enhanced through nano-engineered semiconductor surfaces, improved metal–semiconductor contacts, and plasmonic antennas, which increase charge separation and optical absorption efficiency. Silicon-based PV technologies have evolved alongside halide perovskite photovoltaics, the latter achieving single-junction efficiencies over 26% through improved interfacial passivation, charge carrier lifetimes, and stability, while lowering cost and processing constraints compared to traditional materials.

Nanotechnology also advances ocean wave energy harvesting using nanolayered metals or graphene, which confine charge motion *via* ionic strength gradients. These materials can be deposited onto marine-grade substrates, enabling large-scale integration in coastal infrastructure; however, challenges remain due to corrosive ocean environments and scaling difficulties.<sup>563–565</sup>

In addition, nanomaterials catalyze key chemical reactions essential for sustainable fuel production. Many industrial chemical processes are major greenhouse gas sources; transitioning to reactions powered by electricity rather than combustion is crucial. Nanocatalysts enable sustainable synthesis of hydrogen (H<sub>2</sub>), ammonia (NH<sub>3</sub>), methanol (CH<sub>3</sub>OH), ethylene, propylene, and aromatics, preferably from waste feedstocks.<sup>304–306,562,566,567</sup> Photoelectrochemical cells employing nanomaterials can directly convert solar energy to hydrogen *via* water splitting, enhancing economic viability and environmental sustainability. Plasmonic antenna-reactor nanoparticles catalyze dry methane reforming, converting CO<sub>2</sub> and CH<sub>4</sub>—the two most abundant greenhouse gases—into syngas (H<sub>2</sub> + CO), a precursor for synthetic fuels.

Nanostructuring allows discovery of novel active sites, unique alloy compositions, and improved atom economy through increased surface area-to-volume ratios. Furthermore, understanding nanoparticle behavior under reaction conditions using advanced hardware, software, and AI/ML tools is critical to optimize catalyst performance and accelerate clean energy technologies. Continued research into nanomaterials for energy generation promises significant progress toward a sustainable global energy transition.

**25. How do nanomaterials improve the efficiency of energy storage and transport systems?** Efficient, compact, and reliable energy storage is essential for applications ranging from portable electronics to grid stabilization in renewable energy systems, such as solar and wind.<sup>568</sup> Nanomaterials significantly enhance energy storage technologies, including batteries and supercapacitors, by providing large specific surface areas and tailored nanostructures. These features increase electrode–electrolyte contact,

thereby improving charge rates, storage capacity, and mitigating issues like volume expansion during charge–discharge cycles.<sup>569–574</sup>

Nanoporous materials, including MOFs, zeolites, molecular sieves, and porous carbons, offer vast internal surface areas and tunable pore chemistries, making them ideal for selective storage and controlled release of gases and liquids relevant to fuel storage.<sup>575–585</sup> For instance, MOFs, metal hydrides, carbon nanotubes, and graphene-based materials provide high-capacity, rapid hydrogen absorption and desorption kinetics, crucial for fuel cells in transportation.<sup>586,587</sup> Industrial-scale production of MOFs by companies such as NuMat highlights their commercial viability.<sup>588</sup>

Quantum effects and coupling phenomena within or between nanomaterials open new avenues for system-level improvements in energy storage and conversion.<sup>589,590</sup> Spin-selective processes, exciton–phonon interactions, and exciton-polariton coupling can be engineered to optimize light absorption, carrier extraction, and catalytic activity.<sup>591,592</sup> Nanostructured step edges catalyze bond activation efficiently,<sup>593</sup> and nanoscale optical cavities amplify absorption,<sup>594,595</sup> collectively enhancing photocatalytic and electrocatalytic architectures.<sup>596</sup>

By harnessing these nanoscale phenomena, future energy storage and transport technologies could achieve higher efficiencies, longer lifetimes, and improved integration with renewable energy sources, supporting sustainable energy infrastructures worldwide.

**26. How can nanomaterials address the demand for rare-earth elements amid supply and environmental challenges?** Rare-earth elements (REEs) such as scandium, yttrium, and lanthanum are vital for advanced technologies, including renewable energy devices, electric vehicles (EVs), and high-performance magnets due to their unique electronic, magnetic, and luminescent properties.<sup>597</sup> However, global REE reserves are geographically concentrated—primarily in China, with significant deposits also in Vietnam, Russia, and Brazil—leading to supply vulnerabilities and environmental concerns linked to mining.<sup>598</sup> These challenges drive the need for sustainable REE extraction, separation, and recycling methods.<sup>599</sup>

Nanomaterials offer promising solutions due to their high surface-area-to-volume ratios and tunable structures. Materials such as MOFs, carbon nanotubes, graphene, and nanoscale collectors can be engineered to bind selectively and to extract REEs from ores and electronic waste streams, improving efficiency and sustainability of recovery processes.<sup>600–603</sup> Nanomaterial-enhanced filtration systems can increase separation efficacy in mining and recycling operations.<sup>604–606</sup> Cerium-doped nanocatalysts facilitate material breakdown to improve REE recovery, while bioinspired nanotechnologies utilize mussel-inspired nanocellulose coatings and cyanobacteria for selective REE binding from aqueous media without harmful chemicals.<sup>607</sup> Biodegradable protein-based adsorbents and bionanoparticles are also being developed for sustainable REE extraction.<sup>608,609</sup>

Another strategy is to reduce reliance on REEs by developing alternative materials.<sup>610</sup> AI is being used to guide materials discovery and to accelerate the identification of REE-free or reduced-REE materials. Examples include Zr<sub>2</sub>Co<sub>11</sub> and Fe–Co-based nanoparticle magnets that eliminate REEs, and Pt-REE alloy nanoparticle catalysts designed for lower REE content in hydrogen fuel cells and petroleum refining.<sup>611–613</sup>

These advances promote a sustainable supply chain for REEs critical to modern technology while addressing environmental and geopolitical concerns.

## IMPROVING HUMAN HEALTH AND SAVING HUMAN LIFE

**27. How can nanoscience enhance the well-being and performance of healthy individuals?** Nanomedicine can be used to treat disease and to improve health, performance, and preventive care for healthy individuals.<sup>614,615</sup> A landmark example is the mRNA COVID-19 vaccine, which utilized nanotechnology for effective delivery and immune activation. Preventive medicine, including vaccines, has dramatically reduced infectious disease burdens and certain cancers.<sup>616–618</sup> Structural nanomedicine improves vaccine stability and delivery, enhancing immune responses and minimizing side effects.<sup>619–621</sup>

Nanotechnology also enables performance enhancement in areas such as muscle regulation, sensory augmentation *via* wearable devices, aging delay, and cognitive function improvements through targeted delivery and brain-computer interfaces.<sup>622–624</sup> Gene-editing tools like CRISPR, supported by nanoscale delivery systems, hold potential not only for treating genetic disorders but also for safely modifying biological moieties in otherwise healthy individuals.

Additionally, exogenous wearable, injectable, and inhalable nanosensors facilitate continuous monitoring of physical and cognitive metrics.<sup>625–629</sup> These sensors enable real-time data collection on health, exertion, recovery, and attention, informing personalized optimization strategies in athletics, education, and daily activities. Integration into training regimens and learning environments allows fine-tuning of performance and well-being, enhancing quality of life.

Nanoscience-driven advances in preventive medicine, performance monitoring, and cognitive enhancement offer exciting prospects for improving health and human potential, moving toward a future where technology supports proactive, personalized wellness.

**28. What are the key challenges in developing nanotechnology-based tools for early disease detection?** Nanotechnology promises transformative advances in early, noninvasive disease detection, crucial for timely interventions and patient self-monitoring.<sup>630,631</sup> Effective diagnostic tools require three key components: target recognition, signal transduction, and signal readout.<sup>632–634</sup> Nanomaterials contribute significantly by enabling rapid, sensitive detection beyond symptom-based methods.

Target recognition involves detecting disease-specific molecular markers using highly selective biorecognition elements such as DNA aptamers, spherical nucleic acids (SNAs), and antibodies that bind targets at ultralow concentrations.<sup>635,636</sup> Improving the specificity and stability of these nanoscale and biological components in complex biological fluids is a critical focus for enhancing real-world diagnostic performance.

Signal transduction converts recognition events into measurable signals. Nanoparticles amplify signal strength dramatically, increasing assay sensitivity.<sup>637,638</sup> Therefore, it should be an ongoing research priority to optimize nanoparticle systems to enhance signal fold-change.

Finally, signal readout must provide clear, multiplexed outputs. Nanotechnology enables multiplexed detection *via* quantum dot fluorescence, gold nanoparticle optical contrast,

and other modalities, allowing simultaneous monitoring of multiple biomarkers.<sup>639–641</sup> Increasing multiplexing capacity while minimizing sample volumes remains an important challenge.

Integration of these components into cohesive, reliable diagnostic platforms is essential for clinical adoption. AI-driven design and analysis tools can optimize recognition elements, signal processing, and readout, improving diagnostic accuracy and enabling global healthcare impact. Overcoming these challenges will facilitate the widespread deployment of nanotechnology-enabled early detection tools.

**29. What nanotechnology advances are essential to enable practical point-of-care diagnostics and stable off-the-shelf nanomedicines?** Current antigen-based point-of-care (POC) diagnostic tests, such as those used for COVID-19, still rely on technology developed in the 1960s, for example in pregnancy tests, limiting their sensitivity and applicability.<sup>642</sup> To broaden access to affordable, reliable diagnostics—especially in low-resource settings lacking laboratory infrastructure—advanced POC platforms leveraging nanotechnology are needed.<sup>633,643</sup> Nanomaterials can significantly improve these platforms by enhancing target specificity, amplifying detection signals, reducing power consumption, and minimizing device size, all of which increase portability and practicality.<sup>644,645</sup>

In parallel, developing stable, off-the-shelf nanomedicines that maintain efficacy during long-term storage and transport is crucial.<sup>646</sup> Scalable 3D nanoscaffold biomanufacturing methods offer cost-effective, high-throughput production of engineered cells and nanomedicines that do not require individual personalization each time, thus enabling broader distribution. Self-assembling nanomaterials such as DNA origami-based vaccines provide modular platforms that simplify targeted therapies and reduce the complexity of individualized treatments.<sup>647</sup> Additionally, MOFs have been shown to encapsulate sensitive biologics, creating formulations that withstand shipping and storage stresses without losing potency.<sup>648,649</sup>

Achieving these goals requires close collaboration among nanotechnology researchers, pharmaceutical developers, and healthcare providers. Moreover, clear regulatory guidelines for safety, efficacy, and nanopharmaceutical quality standards are critical to enable widespread adoption. These advances could democratize healthcare by delivering powerful diagnostics and therapeutics directly to diverse populations worldwide, overcoming current infrastructure and supply chain limitations.

## IMPLICATIONS FOR SOCIETY

This Nano Focus has examined how nanoscience and nanotechnology have revolutionized science and engineering—from advances in synthesis to the development of new tools and methods—and how these scientific breakthroughs have translated into technological innovations. We have highlighted key questions across these areas and proposed potential solutions to advance the field. In addition to their direct impacts, nanoscience and nanotechnology have also reshaped broader societal perspectives. The development of novel materials and systems brings unique challenges in areas such as education, ethics, policy, and intellectual property, among others.

## TEACHING NANOSCIENCE AND NANOTECHNOLOGY

**30. How can nanoscience and nanotechnology be integrated effectively into educational curricula and public outreach?** Nanoscience and nanotechnology represent transformative scientific fields with interdisciplinary foundations, making their integration into traditional curricula complex.<sup>650</sup> A key question is whether nanoscience topics should be embedded in existing chemistry, physics, and biology courses, or offered as standalone electives or degree programs, possibly within dedicated nanoscience departments.<sup>651,652</sup> Approaches vary widely, with some institutions focusing on graduate research exposure, while others emphasize undergraduate coursework. Collaborations with industry and government laboratories to align education with workforce demands through internships and cooperative programs have also been explored.<sup>653</sup>

For nanotechnology's economic and societal growth, it is essential to engage learners across educational levels. The U.S. National Nanotechnology Initiative (NNI) promotes workforce expansion *via* public outreach and education, including efforts to introduce nanoscience concepts in K–12 education, which may inspire students and indirectly educate their families.<sup>654–656</sup> Resources include media portrayals (e.g., *Black Panther*, *Ant-Man*), interactive experiences such as Disney World's "Take a Nanooze Break", and educational books.<sup>657,658</sup> However, K–12 curricula often face challenges in accommodating new content due to crowded schedules and limited resources.

Digital platforms are increasingly vital in expanding nanoscience education, with online modules, simulation tools, and remote laboratories providing broader accessibility.<sup>659</sup> Nonetheless, hands-on laboratory experiences remain critical to effective STEM learning. Targeted funding to train teachers and support immersive university-community programs can foster lasting engagement. Partnerships between universities and community or technical colleges are also promising to build a diverse nanotechnology workforce.<sup>655,659–661</sup> These educational strategies aim to cultivate a scientifically literate public and prepare future innovators.

## UNDERSTANDING ETHICAL RESPONSIBILITIES

**31. What are the key ethical challenges posed by nanoscience and nanotechnology, and who should govern their ethical standards?** Nanoscience and nanotechnology raise ethical issues common to emerging technologies: balancing innovation with safety, privacy, and societal impact. However, the rapid pace of development has often outstripped the formulation of ethical guidelines and regulations.<sup>662,663</sup> Future applications—such as nanobots for surveillance, nanoparticle tracers for tracking, or performance-enhancing nanomedicines—introduce complex dilemmas requiring careful ethical scrutiny.<sup>664–667</sup>

Ethical governance should involve the communities affected by nanotechnology, including researchers, policymakers, healthcare providers, and the public, to assess risks and benefits collaboratively. Transparent communication about the potential implications of nanotechnologies is crucial to build trust and enable informed societal decisions. Policymakers must engage the public proactively to educate and to solicit input on ethical standards.

A central challenge is balancing intellectual property protections that incentivize innovation with ensuring equitable

access to nanotechnologies.<sup>668–670</sup> This includes safeguarding privacy while promoting transparency and public benefit. Ethical frameworks must evolve dynamically alongside technological advances, guided by multidisciplinary input and international dialogue to address global impacts. Ultimately, ethical stewardship should enable responsible innovation that maximizes societal benefit while minimizing harm.

## INTEGRATING NANOSCIENCE AND PUBLIC POLICY

**32. What are the main public policy challenges for nanoscience, and how can global coordination enhance regulation and innovation?** Nanoscience and nanotechnology have become integral to many commercial products, from quantum dot TVs (Samsung, Sony) to lipid nanoparticle drug delivery systems (Evonik) and advanced materials (DuPont, BASF).<sup>671</sup> Regulatory frameworks differ by region; in the U.S., the FDA regulates many nanomaterials, while Europe applies REACH regulations with member states overseeing compliance.<sup>672–674</sup> These frameworks ensure safety but can fragment risk assessment and market access, complicating global exchange.

Global coordination is essential to harmonize regulations, reduce trade barriers, and create consistent safety standards. International bodies such as the International Organization for Standardization (ISO), the Organisation for Economic Co-operation and Development (OECD), and the World Health Organization (WHO) play key roles in developing and updating global regulations and testing protocols for nanomaterials.<sup>675–681</sup> Policies must be adaptive as new materials with novel properties emerge, addressing classification, handling, disposal, and recycling challenges.

A responsible policy approach also requires assessing long-term environmental and health impacts. For example, while heavy metal nanoparticles like those containing lead or mercury pose toxicity risks, they remain critical for applications like catalysis and imaging.<sup>674,682,683</sup> Balancing these risks with benefits is a continuous regulatory challenge. Ultimately, coordinated global policies can foster innovation while protecting public and environmental health, enabling nanotechnology's sustainable integration into economies worldwide.

## INTEGRATING NANOSCIENCE AND NANOTECHNOLOGY WITH INTELLECTUAL PROPERTY

**33. How can intellectual property (IP) frameworks support nanomaterial innovation while ensuring broad societal benefit?** Balancing open innovation with protecting proprietary discoveries is vital for advancing nanoscience and translating research into public benefit. Nanoscience generates vast data sets describing material properties and interactions across various environments, often produced *via* high-throughput experiments and theoretical models.<sup>684</sup> Both AI and ML accelerate discovery by analyzing trends and optimizing materials for specific uses.<sup>685–687</sup> However, sharing data widely while protecting IP poses a significant challenge.

Adoption of FAIR principles (Findable, Accessible, Interoperable, Reusable) for data management promotes accessibility and reuse of nanomaterial data sets.<sup>688</sup> Emerging IP frameworks may require clear documentation of human input in AI-assisted inventions to ensure patentability without stifling collaboration. A hybrid model may evolve where foundational data remains open, while specific, application-driven innovations receive patent protection.

Bridging fundamental research and commercial application needs new funding structures and policies encouraging precompetitive collaboration. Public-private partnerships can facilitate data sharing while preserving rights necessary for market entry. Supporting environments that foster open science alongside attractive IP protections will accelerate innovation and maximize societal impact. In sum, thoughtful IP management is key to unlocking nanotechnology's full potential, balancing innovation incentives with broad access and societal benefit.

## SUMMARY AND OUTLOOK

Although the questions have been grouped by themes—foundational understanding, tools and techniques, impactful applications, and societal implications—the responses reveal the deep interdependence and interdisciplinarity of these areas. Several key themes have emerged. Nanoscience and nanotechnology will advance significantly as we move closer to 1) Achieving atomically precise nanoparticles and nanostructures and gaining the ability to analyze, understand, and control their composition over time—similar to how we write and manipulate chemical reactions for molecules; 2) Developing *in situ* and *operando* characterization tools for single particles and structures, shifting from ensemble-averaged data to atomistic insights, as is possible in many molecular systems; 3) Using the nanoscale as a true bridge between the quantum and macro scales—understanding transitions across scales, controlling properties within a single system, and producing materials at scales relevant to real-world applications; 4) Leveraging AI and ML to accelerate all aspects of the field, from discovery and synthesis to application; and 5) Enhancing public understanding, societal integration, and global collaboration—recognizing that if chemistry is the “central science,” then nanoscience and nanotechnology may well be the “central” central science. In summary, by posing and addressing 33 key questions in nanoscience and nanotechnology, we have established a framework to inspire and to guide future research across the field.

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## Notes

The authors declare the following competing financial interest(s): A.H.S. is a shareholder of Exicure Inc., which develops SNA therapeutic platforms. A.H.S. is an inventor on patent US20150031745A1, which describes SNA nano-conjugates that cross the blood-brain barrier. V.P.D. is co-founder of Coral Innovations, a nanotech start-up that is commercializing IP on water cleanup from NU. C.A.M. has financial interests in Azul 3D, Inc., TERA-print, LLC, Mattiq, Inc., and Flashpoint, Inc., which could potentially benefit from the outcomes of this research.

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