

Engineering Next-Generation Hybrid Nanomaterials, From Advanced Sensors to Sustainable Catalytic Processes

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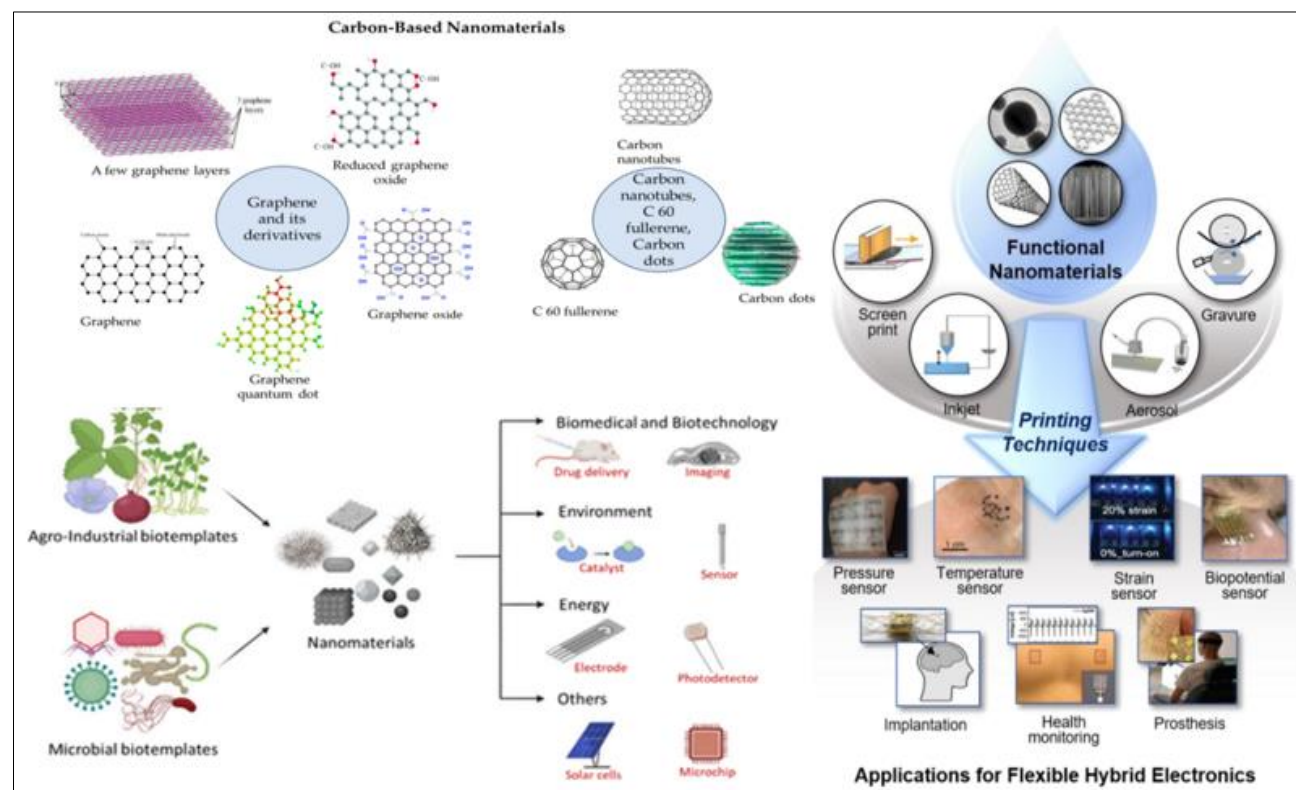
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Abstract



The hybrid nanomaterials represent a revolutionary type of engineered structure that lies on the boundary of the chemistry and materials science and nanotechnology. With a combination of discrete organic-inorganic, metallic-polymeric, or bio-inspired constituents at the nanoscale, the systems are strongly synergistic in terms of physicochemical properties, and by far outperform their individual components. This structural and functional tunability has provided new opportunities in

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sensor technology, energy conversion and sustainability in catalysis that has never been seen before. Recent progress in interfacial design, atomic-level assembly, as well as nanoscale characterization, have made it possible to highly tune charge dynamics, surface reactivity, and selective molecular recognition. In sensor devices, the hybrid nanomaterials have excellent sensitivity and signal fidelity due to the property of the designs of heterostructures engineering and quantum confinement. Likewise, their hierarchic structures and functional active sites enable efficient energy capture, pollutant reduction as well as green chemical reactions in catalytic systems at ambient conditions. The overlap between artificial intelligence, computational modeling and green synthesis protocols is also rapidly increasing the rational designing of hybrid nanomaterials to be used in sustainable technology applications. It is a review that critically evaluates the new synthesis strategies, structure-property correlations, and multifunctional uses of next-generation hybrid nanomaterials, and shows the progress along with the unfulfilled opportunities of providing scalable, environmentally responsible production. Lastly, the future directions are suggested to a new paradigm of adaptive, circular-economy-oriented design based on integrating efficiency, durability, and ecological compatibility in the state-of-the-art materials engineering.

Keywords: Hybrid Nanomaterials, Interfacial Engineering, Sustainable Catalysis, Nanosensors, Green Synthesis, Synergistic Heterostructures, Energy Conversion.

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1. INTRODUCTION

The unceasing development of the materials science has been significantly influenced by the goal of miniaturization and multifunctionality and has led to the development of innovation not only in bulk systems but also in nanoscale structures (Ariga *et al.*, 2021). In this sense, hybrid nanomaterials have become one of the most vibrant frontiers with an unparalleled control over matter by means of purposeful assembly of discrete components that act synergistically. This idea of hybridization transcends the conventional materials design in that it integrates the various phases and organic and inorganic, metallic and polymeric or biologically inspired and synthetic into the conclusive forms with highly fine-tuned interfaces (Nicole *et al.*, 2014). These architectures exploit the synergies in the nanoscale where interfacial effects dominate the total performance and, consequently, new paradigms in the sensing, catalysis, and energy conversion are reinvented (Yang *et al.*, 2018).

The global trend of shifting to sustainable technologies has helped the further speed up of the search of the materials which would guarantee a superior performance with less impact on environmental costs (Tiwari *et al.*, 2023). The flexibility in terms of compositions that can be customized and functionality that can be adjusted makes hybrid nanomaterials versatile in the sense that they provide a versatile platform of accomplishing such objectives. Their architecture is capable of performing the optical, electrical and catalytic behaviors in a controlled way by manipulating the heterostructure engineering and interfacial charge. To illustrate, the integration of plasmonic metals with semiconductors can improve the light-matter and charge carrier separation which are essential in photoelectrocatalysis and pollutant degradation (Yu *et al.*, 2019). In a similar vein, the combination of the conductive polymer and metal-organic frameworks (MOFs) or the carbon-based substrates improves sensor responsiveness, flexibility, and biocompatibility. Therefore, the hybrid nanomaterials serve as convergent platforms that enable the integration of the principles of chemistry, physics,

and engineering to answer the urgent problems of energy and the environment (Gupta *et al.*, 2022).

Scientifically, the hybridization strategy exploits the property of complements. Structural rigidity, high thermal stability, and electronic conductivity is normally provided by the inorganic domains, whereas various flexibility, chemical selectivity, and processability is provided by organic or polymeric phases (Li *et al.*, 2023). This duality leads to hierarchical order materials, defect-controlled interfaces and surfaces with customized surface chemistries, which allows highly directional functional capabilities. The interaction between these two different realms is critical in determining transport of charges, kinetics of adsorption and catalytic turnover rates. As a result, surface functionalization, dopant integration or atomic level patterning of interfacial engineering has emerged as a theme in the rational design of hybrid nanostructure (Liu *et al.*, 2012).

The current technological changes are radically transforming the conceptualization and optimization of hybrid nanomaterials (Huang *et al.*, 2014). However, predictive modeling of structure-property relationships has become possible now with the assistance of artificial intelligence (AI) and quantum-based simulation, which streamlines the creation of materials with functionalities of interest prior to their actual experimental production. Large-scale computational screening enables the search of large compositional space to accelerate the identification of hybrid systems with desirable electronic band structure or adsorption energies. Parallel to this, the manufacturing of nanomaterials is being made less ecologically impactful by green synthetic methods, solvent-free reactions, supercritical fluid handling and bio-templated growth. Such sustainable approaches are important in the process to align nanotechnology with the idea of the circular bioeconomy and the United Nations Sustainable Development Goals (Kumar *et al.*, 2024).

The field of use of hybrid nanomaterials is truly vast and growing. In the next generation sensors, such hybrid structures allow both high selectivity and fast response by taking advantage of the synergistically

relevant behavior between conductive, catalytic, and adsorption-active spaces (Qu *et al.*, 2025). Examples of hybrids on metal, oxide and graphene include degree of high surface area and high electron movement, resulting in sensors that can detect trace gases or biomolecules down to the sub-ppm level. Hybrid nanomaterials in photocatalytic and electrocatalytic systems enable the realization of the solar-to-chemical energy conversion process with high efficiency through the establishment of the charge separation at properly aligned heterojunctions. These systems play a central role in hydrogen evolution, CO₂ reduction and pollutant remediation systems. In addition to these, hybrid nanomaterials are the basis of developments in the energy storage technology, including batteries and supercapacitors, where their interfacial controllability provides high capacity, cycling stability, and ion transport efficiency (Dubal *et al.*, 2015).

In spite of such impressive progress, there are still a number of issues that hamper the full scale application of hybrid nanomaterials (Hodges *et al.*, 2018). Molecular Control of interface chemistry on the atom level is a very difficult challenge, especially in heterogeneous composite systems where substances are dynamically interacting. Scalability, reproducibility and long-term stability problems also remain, which makes it difficult to move the laboratory synthesis to an industrial manufacturing process. Also, the sustainability of hybrid nanomaterials in life-cycle including its recyclabilities, environmental persistence and its toxicities must be systematically evaluated. They are imperative in ensuring that the manufacturing of sophisticated materials is sustainable rather than part of the dumping of wastes in the future (Nizam *et al.*, 2021).

To overcome these restrictions, interdisciplinary strategies in which materials informatics, in situ characterization and eco-design principles are integrated are required. Recent technologies, such as operando spectroscopy, electron tomography, machine-learned optimization of synthesis are providing deeply insightful information into the dynamic programming of the evolution of hybrid interfaces in operating conditions. Such information-centered approaches will almost certainly bridge the knowledge gap that exists between the functional performance and material design (Mellal *et al.*, 2024). The review is aimed at summarizing scientific progress that has been made in the recent past concerning the development of hybrid nanomaterials with particular reference to their use in advanced sensing and sustainable catalytic uses. Furthermore, it also tries to outline design directions next generation as an effort to control the interface, scale synthesis, and integration towards the circular economy in an effort to streamline the sustainable development of hybrid nanotechnology.

2. Convergence at the Interface, Synergistic Design Principles of Hybrid Nanomaterials

The remarkable performance of hybrid nanomaterials can be found at their interfaces, where the dissimilar phases meet each other to provide emergent properties that cannot be produced by the solitary components (Zhang *et al.*, 2018). This interface space serves as an active stage of charge redistribution, energy transfer and structural stabilization to regulate the overall material performance across a spectrum of applications including ultrasensitive sensors to high-efficiency catalyst systems. The development of hybrid nanomaterials is therefore determined by the ability to control interfacial reactions on an atomic, molecular and mesoscale where chemical compatibility and electronic coupling determine the resulting synergy.

2.1. Architectures of Hybrid Interfaces

The basic principle of hybrid nanomaterial engineering consists of precise assembly of metalorganic, polymericinorganic and covalentheterostructure interfaces. The atomic level control of bonding arrangement and lattice continuity is determined by the degree of orbital overlap and defines how quickly charge is transported across the interface (Sood *et al.*, 2021). One such example is metal-organic frameworks (MOFs) of coordination which form channels of selective electron transfer, and covalent labeling of organic substrates to the surface of semiconductors stabilize excitonic states and prevent carrier recombination. The surface chemistry of each constituent of each functional group, oxidation state, and defect density are essential to the design of interfacial dynamics of charge transfer. Even though lattice mismatch is often considered to be a source of stress, this mismatch may be utilized to trigger localized electronic perturbations, which may be employed to catalyze catalytic turnover or selective sensing. The structure coherence at the junction, thus, ought to be optimized to capitalize on the defect formation of the strain against quantum-level energy level coupling to attain optimum reactivity and sensitivity (Jooss *et al.*, 2025).

2.2. Quantum Coupling and Energy Transfer Mechanisms

On the nanoscale, quantum coupling effects control interfacial synergy by hybridizing different electronic states resulting in band realignment, electron tunneling and energy delocalization across heterojunctions. The development of the interfacial dipole also changes the local potential differences, increasing the velocity of charge separation and directional movement of electrons. Hot electrons produced by surface plasmon resonance in a plasmonic semiconductor system, such as in plasmonic nanoparticles, may be used in catalysis reactions or in photodetection applications (Khan *et al.*, 2015). Likewise, there is the transfer of energy in bio-synthetic hybrids, which utilize Förster and Dexter mechanisms to control photoluminescence and charge migration. The

extrinsic evidence of transient charge polarization and ultrafast relaxation reactions has been directly observed through advanced in situ operando spectroscopic studies and proved that performance improvement in hybrid materials is not only due to the addition of the components, but also emergent quantum coherence at the interface. The strategy of controlling such a coupling by means of chemical modulation and nanoscale alignment continues to be a leading approach to improving sensor accuracy as well as catalytic likeness (Jambhulkar *et al.*, 2020).

2.3. Defect and Disorder as Design Tools

In opposition to the old-fashioned quest of crystal-like perfection, controlled defect engineering is nowadays employed as a deliberate approach of tuning of hybrid nanomaterial functionality. Vacancies, dislocations, and heteroatomic substitutions are active centers that determine the energetics of adsorption, redox potential, and carrier mobility (Zhang *et al.*, 2025). Surface vacancies in catalytic hybrids ensure the adsorption of oxygen or hydrogen and in effect reducing activation barriers to conversion reactions. On the same note, optical bandgaps can be modulated with local states, due to defects, to extend light absorption to the visible or near-infrared spectrum of light, and with increased photoactivity. The new dichotomy between stochastic and deterministic defect models which is able to offer complementary solutions to the same problem is the promotions of entropy-driven surface reactivity by random defect distribution and predictable electronic state manipulation by deterministic insertion of individual dopants. Learning to balance between order and disorder is thus an excellent framework of customizing catalytic reaction strategies and sensing properties without impaired material stability (Shen *et al.*, 2021).

2.4. Predictive Modelling and AI-Driven Interface Design

The increasing sophistication of multi-component systems has fostered the merging of machine learning (ML) and data-driven modelling to forecast the results of interfacial stability, energy alignment and performance. Algorithms that are trained on high-throughput data sets are able to discover previously unrecognized correlations between the synthesis

conditions and structural configurations to facilitate inverse design frameworks, whereby desired functionality informs not the composition of materials, but vice versa. Sophisticated simulations based on ML-assisted molecular dynamics and density functional theory (DFT) have become the ability to accurately predict interfacial distributions of charge densities, adsorption energies, and band offsets and relieve the empathetic trial and error pressure by a significant margin (Liao *et al.*, 2022). With these predictive paradigms, scientists are in a position to computationally chart hybrid nanomaterial landscapes to identify the most favorable combinations of elements and production paths, which generate the greatest interfacial synergy. Such intersection of artificial intelligence and quantum chemistry will be a critical advancement of descriptive into prescriptive material design and will speed up the innovation in future-generation nanosystems.

2.5. Translational Pathways: From Theory to Device Fabrication

One of the most prominent problems in the research on hybrid nanomaterials is filling the gap between theory and practice. The reproduction of synthesis is not sufficient to be done successfully in translation, a good translation requires integrity of the interface in the scale-up and integration of the device. Hybrid MOFs on conductive surfaces in gas sensing applications exhibit a thermo-adjustable porosity and amplification of signal, and the atomic-level design is transformed into selectivity and sensitivity in reality. On the same note, plasmonic semiconductor catalysts combine photothermal conversion and charge-driven reactivity to provide better solar-to-chemical efficiencies. However, scaling puts complexities on these architectures (interlayer delamination, non-uniform dispersion, and interface degradation during operational conditions) (Wen *et al.*, 2024). New nanomanufacturing methods are available, such as self-assembled monolayer deposition, atomic layer epitaxy, and additive nanoprinting, which provide ways of preserving nanoscale fidelity to macroscopic devices. The final goal is to create manufacturable hybrid platforms that do not compromise interfacial accuracy so that the theoretical potential of nanoscale synergy is completely fulfilled by the practical and sustainable technologies.

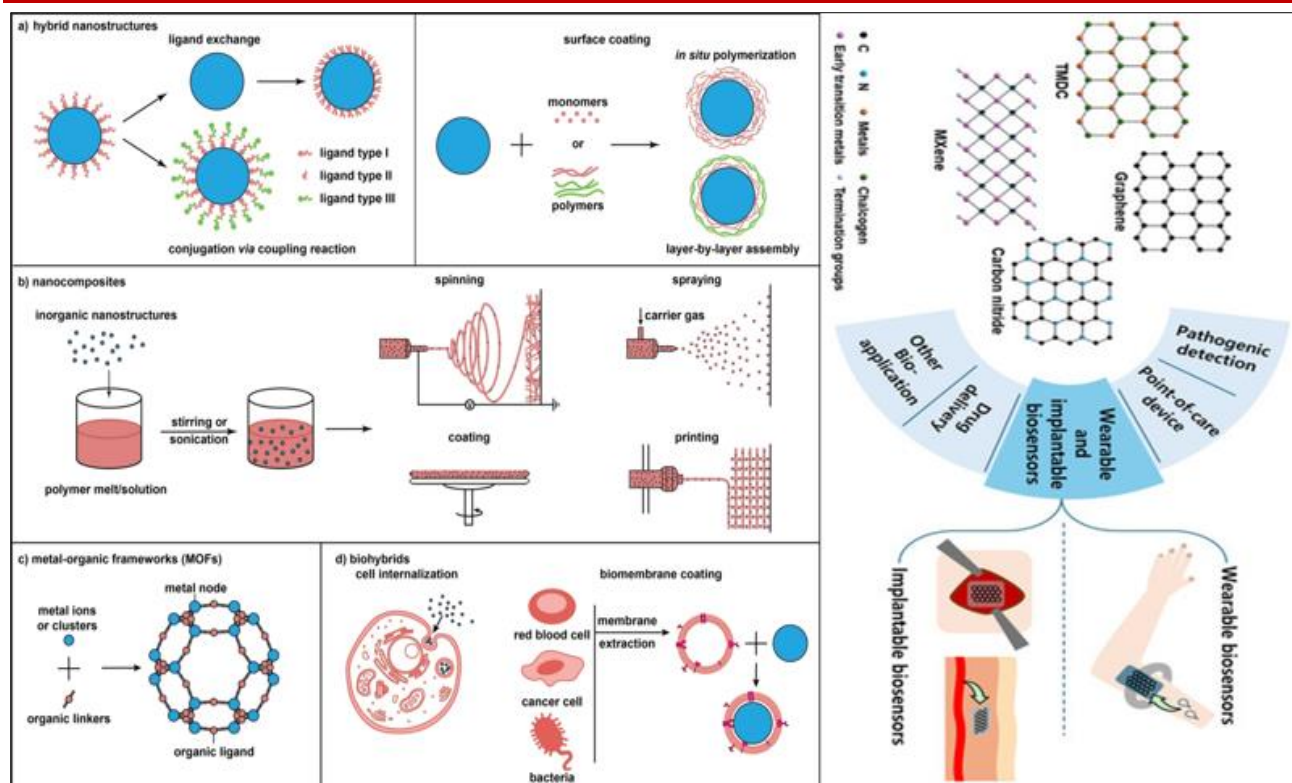


Fig. 1: Convergence at the Interface, Synergistic Design Principles of Hybrid Nanomaterials

3. Beyond Functionality, Bioinspired and Biohybrid Nanomaterials for Sensing and Green Catalysis

The convergence of biology and nanotechnology has introduced a new paradigm of transformation in which the principles of natural design are applied and novel biohybrid nanomaterials are developed that combine the capability of catalytic specificity and environmental flexibility with the need to be environmentally acceptable. These systems extend the traditional material limits by combining the biological components, including enzymes, proteins, cells, or biomacromolecules with an inorganic or synthetic matrix to restore the efficiency, specificity and sustainability of living systems. Bioinspired nanomaterials are driven by the ecological logic unlike traditional hybrids which are only driven by the performance metrics and desired harmony between molecular functionality and environmental stewardship (Chakraborty *et al.*, 2023). In this field, sensing and catalysis can be considered a point of focus, where biomimicry can provide highly selective, energy-efficient, and self-sustaining technologies.

3.1. Lessons from Nature: Enzymatic and Cellular Models

Nature has offered the best blueprint of functional complexity with hierarchical structure of biological composites like shells, bone, and photosynthetic membranes. Such structures have multiscale incorporation of atomic accurateness in active places and mesoscale porosity and macroscopic stability leading to impressive effectiveness in energy transduction and molecular recognition. An example of such synergy is enzymes, which facilitate catalytic

changes with active pockets set up, specific binding and conformational flexibility. It has been hoped that translating these molecular recognition and selectivity principles into artificial biomaterials would inspire the design of artificial enzymes, or nanoenzymes, that behave like biocatalysts but with increased stability in unfriendly conditions (Wu *et al.*, 2019). In equal measure, cellular architecture offers concepts of compartmentalization and control of transport which informs the design of nanostructured scaffolds that can channel substrates and spatially resolved reactivity central characteristics to advanced sensors and catalytic reactors.

3.2. Biomimetic Synthesis Pathways

In a bid to follow the path of biological efficiency, scientists have resorted to biomimetic and bioinspired synthesis pathways that favor environmental innocence and resource circularity. Biofabrication Techniques to use biological molecules or organisms as structural guides and catalysts in material assembly include biotemplating, enzymatic mineralization and hydrothermal biofabrication. As an example, inorganic nanoparticles with directed morphology and crystallinity can be nucleated using peptide or polysaccharide templates, whereas room-temperature synthesis can be done with enzymatic pathways using non-toxic reagents. In addition to being environmentally friendly, the techniques also provide the ultimate morphological control and surface functionalization, which allows access to the active sites to fine-tune their reaction. Circular economy concepts are even integrated further in the design of nanomaterials by the introduction of waste

valorization strategies, which include using biomass residues, agricultural by-products, or fish-derived proteins as precursors (Maschmeyer *et al.*, 2020). Green chemistry and biotechnology merge to create a platform of sustainable hybridization by lessening the environmental footprint and the cost of production.

3.3. Biohybrid Sensors and Catalysts

Biological recognition systems when combined with inorganic platforms have produced biohybrid sensors of unprecedented sensitivity and selectivity. An example of this strategy is enzyme-nanoparticle conjugates, in which enzymes are immobilized on conductive/plasmonic nanoparticles to increase kinetics of electron transfer without affecting biocatalytic selectivity, allowing detection of trace analyte, including glucose, toxins or environmental pollutants. Likewise, both DNA and antibody-functionalized nanocomposites take advantage of molecular recognition to realize sub-nanomolar limits of detection. By extension, biohybrid devices that are self-regulating and based on the integration of microbial cells and nanoscale conductors or catalytic particles are achieved through the introduction of living-material systems (Kim *et al.*, 2024). Such microbial nanoparticle interfaces can also be sensed in situ and catalyzed, with metabolic activity driving redox reactions or pollutant breakdown. These constructs disenclose the line of differentiation in the realms of biology and synthetic engineering and show self-sufficient performance and adaptive responsiveness within a shifting environmental set-up.

3.4. Dynamic Self-Regeneration and Adaptivity

Another characteristic characteristic of a biological system is the ability to repair itself and behave adaptively, which is being replicated in the next generation of hybrid materials. Responsive polymers, enzyme cascades, or redox-active biomolecules can be

used as biohybrid nanostructures which can be autonomously regenerated to catalyze or sense again after degradation. Enzyme-metal oxide complexes as an example can rebuild active states by reacting to substrate depletion or environmental pressure via feedback. In a similar manner, the adaptive nanostructures can be tuned to have a porosity, hydrophobicity, or charge distribution with pH, temperature, or light and remain stable in operations under varying conditions (Shao *et al.*, 2025). These self-regulating qualities increase material life, reduce maintenance and are congruent with the philosophy of sustainable material intelligence in which hybrid systems resemble the resiliency and homeostasis of biological systems.

3.5. Toward Sustainable Industrial Applications

It is the combination of biohybrid nanomaterials in large-scale sustainable processes in catalysis and detection that is needed to transition the technology to the industrial world. Bioinspired catalysts based on metalloenzyme motifs show high selectivity towards formate or methanol, which makes them much more energy-efficient and purified products than traditional metallic catalysts in the generation of CO₂. In the same manner, biohybrid photocatalysts based on photosystem-mimetic chromophores on semiconductor supports allow CO₂ and water to be converted into fuels of value by using solar energy. Enzyme-immobilized nanofibers and biofunctionalized membranes are used in the wastewater treatment process to degrade pollutants with low toxicity and can be recycled (Al-Maqdi *et al.*, 2021). Comparative life-cycle analyses show that these biohybrid systems save energy requirements by a large margin and formation of hazardous by-products by a large margin as compared to the traditional counterparts. The future remains in the creation of scalable models of manufacturing and modular reactor designs that capture bio-accuracy in strong, industrialized models.

Table 1: Bioinspired and biohybrid nanomaterials combine natural design engineering functionality to provide sustainable, adaptive and high-performance sensing and catalysis systems. These are important biological inspirations, the synthesis pathways, and eco-efficient mechanisms that drive the next-generation green nanotechnologies as highlighted in this table

Dimension / Focus Area	Natural or Biological Inspiration	Bioinspired / Biohybrid Design Strategy	Functional Outcome (Sensing / Catalysis)	Sustainability and Adaptivity Features
Enzymatic Catalysis Models	Enzyme active sites, substrate specificity, dynamic conformational control	Nanozyme design mimicking active-pocket geometry and electron channeling	Enhanced catalytic turnover, pollutant degradation under mild conditions	High stability, self-regeneration of catalytic sites
Cellular and Compartmental Blueprints	Cellular organelles enabling spatial control and substrate channeling	Nanostructured scaffolds for compartmentalized reactions	Improved selectivity and efficiency in cascade catalysis	Adaptive transport and self-repair under stress
Biomimetic Synthesis Pathways	Biogenic mineralization and template-directed growth	Peptide- or polysaccharide-assisted nanoparticle nucleation	Controlled morphology and surface reactivity for sensor interfaces	Low-energy synthesis, use of biomass precursors, circular economy alignment

Dimension / Focus Area	Natural or Biological Inspiration	Bioinspired / Biohybrid Design Strategy	Functional Outcome (Sensing / Catalysis)	Sustainability and Adaptivity Features
Enzyme–Nanoparticle Conjugates	Enzyme–substrate binding coupled with redox activity	Immobilized enzymes on conductive or plasmonic nanoplatforms	Ultra-sensitive detection of glucose, toxins, or pollutants	Renewable biocatalyst interfaces with recyclability
DNA/Antibody Functionalized Systems	Molecular recognition in immune or genetic mechanisms	DNA or antibody-modified nanocomposites	Sub-nanomolar sensing of biological or environmental targets	Biocompatible, recyclable biosensing matrices
Living Biohybrid Systems	Microbial metabolic redox reactions	Microbe–nanoparticle hybrid reactors	Self-powered pollutant degradation and biosensing	Autonomous operation, self-sustaining metabolic cycles
Dynamic Self-Regenerating Materials	Biological tissue repair and homeostasis	Responsive polymers and redox-active biomolecules	Restoration of catalytic and sensing activity post-degradation	Self-healing, prolonged operational lifespan
Sustainable Industrial Deployment	Ecosystem efficiency and circular metabolism	Scalable green fabrication using waste valorization	Industrial sensors and catalysts for CO ₂ reduction, wastewater treatment	Closed-loop material life cycle, minimal ecological footprint

4. Digital Nanomaterials Engineering, Data-Driven Design and Autonomous Discovery

Artificial intelligence (AI), computational chemistry, and autonomous experimentation have shifted the direction of hybrid nanomaterials studies, changing it to data-driven discovery instead of empiricism. This is a digital revolution and fast way of using it is to explore large areas of compositional and structural space, reducing the gap between idea and realization of advanced nanomaterials drastically. With predictive modelling, robotic synthesis, and real-time analytics, researchers are creating a novel paradigm of digital nanomaterials engineering, whereby design accuracy, scaling and sustainability meet in cyber-physical environment (Parizad *et al.*, 2025).

4.1 Data Infrastructures for Hybrid Nanomaterials

Data-centric nanoscience is based on the creation of FAIR (Findable, Accessible, Interoperable, Reusable) data infrastructures that can meet the multidimensional complexity of hybrid systems. These databases capture the atomic configurations, synthesis parameters, surface energetics and catalytic descriptors of a wide range of hybrid architectures allowing systematic pattern recognition and cross-domain inference. Digital twins virtual replicas of real-life systems can be considered the extension of this framework, where the simulated and experimental data can be continuously synchronized. This has been made possible by the combination of high throughput computational pipelines, where a researcher can automate the calculation of surface energies, adsorption geometries, and reaction pathways that can reveal structure-property relationships that can be used to optimize the material. Such interrelated data ecosystems turn materials discovery by the isolated experiment and

make it a networked and global intelligence system which changes every time a new dataset is added (Batra *et al.*, 2021).

4.2. Machine Learning in Property Prediction

Machine learning (ML) has now turned into an essential instrument of uncovering the nonlinear relations that dictate the performance of hybrid nanomaterials. Deep generative neural networks (including variational autoencoders and graph neural networks) can sample hypothetical catalysts with a desired surface topology and active site geometry that optimize desired reactivity or stability measures. In the meantime, transfer learning systems rely on the information obtained in highly characterized materials to improve the predictive power in new or data-deficient systems especially useful in the optimization of sensing selectivity or adsorption selectivity in complex mixed matrices (Viswanathan *et al.*, 2022). ML models allow the mapping of electronic descriptors, orbital interaction, and charge transfer parameters to experimental results which might be catalytic turnover frequencies or detection limits. This predictive capability allows investigators to create materials whose functioning can be known in advance prior to synthesis to reduce wastage and speed up innovation.

4.3. Self-Driving Laboratories and Robotic Synthesis

The advent of automated laboratories is an important step towards self-discovering materials. These platforms combine robotics and AI-based decision algorithms with in situ characterization tools in closed feedback loops that refine synthesis conditions iteratively based on performance metrics. Robotic combinatorial reactors are capable of producing hundreds of hybrid nanostructures with both

composition or morphology gradients and real-time spectroscopic monitoring and electrochemical analysis provide data input back to the AI controller to optimize. This experimental paradigm is a closed loop that replaces workflow in traditional trial and error models by a self-corrective process in which one step in the process informs the next, which accelerates by large multiplied the throughput and reproducibility of the work (Zhu *et al.*, 2025). The integration of robotics and intelligent control, in turn, allows to screen complex hybrid architectures combinatorically, revealing the best compositions and interfaces faces, with little human input.

4.4. Multiscale Simulation of Hybrid Interfaces

The behavior of hybrid nanomaterials is forced to be comprehended and anticipated through the application of computational tools that may mediate the electronic, atomic and mesoscale phenomena due to the complexity of the problems. Multiscale simulation frameworks are quantum mechanical simulations that complement continuum-scale simulation models with accuracy to offer a quantitative description of the interactions between charge carriers and lattice vibrations and reactions at the surface. The quantum and continuum correlation can provide information on the interfacial charge dynamics, dielectric screening and a defect-mediated process that defines the catalytic and sensing efficiency (Muhammad *et al.*, 2024). The new trends in hybrid DFTML pipelines unify the precision of the density functional theory with the performance and flexibility of machine learning and allow predicting the adsorption energetics of the band alignments and transition-state energetics of extremely large chemical spaces with high-fidelity. These simulations do not explain mechanistic paths only, but also feed-back to AI models, making them more predictive, depending on learning physics.

4.5. Cyber-Physical Integration in Smart Manufacturing

The establishment of cyber-physical manufacturing ecosystems, in which real and virtual processes are under continuous synergy, is the finishing point of digital nanomaterials engineering. Synthesis reactor and deposition system digital twins allow real-time monitoring of the processes, adaptive control and scaling of hybrid nanomaterials in a predictive manner. Combining sensor data, process analytics, and ML-driven prediction, a manufacturer is able to maintain the same quality of products and reduce energy usage and material costs. Predictive maintenance algorithms also make nanofabrication elements more reliable by detecting derailment or wearage before the part breaks and maintaining continuous performance and consistent quality of the batches (Sharmile *et al.*, 2025). The combination of computation, automation, and materials science is the basis of the new understanding of smart nanomanufacturing, in which each step of the atomistic

design to industrial implementation is optimized digitally.

5. Quantum–Plasmonic Hybrid Systems, Redefining Limits in Sensor Sensitivity and Catalytic Selectivity

The combination of quantum physics and the study of plasmonic nanoscience has led to the emergence of a new generation of quantum-plasmonic hybrid materials that have the potential to manipulate the light-matter interaction at a highly fine scale. These systems realize the classical performance of both sensors and catalysts by harnessing the quantum confinement of low-dimensional materials coupled with the collective actions of surface plasmonics to exceed the lowest attainable sensor sensitivity and selectivity of catalysts (Zhou *et al.*, 2025). The resulting architectures are dynamical as opposed to passive photonic-quantum interfaces in which energy transduction, charge migration and optical field confinement occurs in coherently coupled regimes. This type of synergy is through which hybrid materials are changing the fundamental thresholds of chemical detection, light-driven catalysis and quantum-enabled conversion of energy.

5.1. Quantum–Plasmonic Coupling in Hybrid Architectures

The basic issue of quantum emitters and plasmonic nanostructures on the interface of the latter is defined by a correlation between the strength of the interaction and the functional activity and the mechanism. Plasmonic fields have the ability to enhance local electromagnetic strength in weak coupling regime and accelerate that of molecular excitation and charge exchange without altering the state of energy. Strong coupling regime on the other hand, plasmonic and quantum modes are coupled in the strong coupling regime to form new quasiparticles plasmon-exciton polaritons, which change the electronic density of states and restructure catalytic landscapes (Xiang *et al.*, 2024). These consistent interactions are what lead to nonthermal breaking of chemical bonds that enable the catalysis of chemical reactions with catalysts being quantum coherence-assisted, and delocalized electronic oscillations lower activation barriers, as well as control reaction selectivity. The capability to manage such coupling, which is dictated by the particle-particle distance, dielectric environment in the surrounding and density of quantum emitters is the core of the next-generation plasmonic hybrids that will be on the interface between photonics and chemistry.

5.2. Hot-Electron Dynamics and Photocatalytic Enhancement

Hot electrons generation and manipulations are the fundamental centers of plasmon-enhanced catalysis and detection. Vibrant carriers with the ability to produce redox changes, or control interfacial charge densities can be generated when damping of corporal movements of the electrons in plasmonic nanostructures when absorbing light. In ultrafast charge carrier injection in

hybrid structures, charge carrier injection occurs in response to plasmonic metal injecting charge carrier into neighboring semiconductors or molecular adsorbates and catalyzing reaction pathways which would have been thermodynamically prohibited in ground-state chemistry. The dynamics of relaxation of these carriers caused by electron-phonon interactions, defect scattering and interfacial orientation determine quantum yield and reaction efficiency. These processes have since been mapped in time with a sub-picosecond resolution with femtosecond transient absorption spectroscopy and time-resolved photoemission displaying oscillations of coherent charges and tunneling processes intervening optical excitation with chemical reactivity (Zhang *et al.*, 2025). Hot-carrier lifetimes can be controlled with control over the morphology of nanoparticles and dielectric confinement, and maximization of energy transduction efficiency can be directed towards a specific photocatalytic reaction, e.g. CO₂ reduction, hydrogen evolution or pollutant degradation.

5.3. Photonic Band Engineering and Nanoantenna Design

Nanoscale optical confinement requires photonic band engineering to control the light propagation, localization and resonance. Nanoplasmonic Systems Hybrid quantum-plasmonics systems apply nanoantennas geometries, periodic gratings and multilayered metastructures to compare the electromagnetic fields and spectral response. The optimization of optical modes to sub-molecular sensing with geometry variation and variation in the gap distance and dielectric composition of optical modes can enable single biomolecule label-free optical mode sensing at single molecules or in the gas-phase. Wavelength-selective resonances are applied in catalytics to enhance light absorption as well as charge excitation within a smaller spectral range to selectively activate a certain chemical bond (Lu *et al.*, 2021). This amount of control is not limited to factors of enhancement and as such, researchers can develop hybrid materials with photonic memory, where resonant states may store and dissipate energy dynamically time in response with reaction cycles. The possibility to compute the optical density of the states in the atomic scale reshapes the operating limits of photoactive nanomaterials.

5.4. 2D Materials as Quantum-Plasmonic Modulators

Graphene and transition metal dichalcogenide (TMDCs), and black phosphorus are two dimensions (2D) materials that have presented a new plasmonic engineering liberty. They are the most quantum-plasmonic modulators, carrier mobility is superb, atoms are atomic, are able to be tuned in band structure, and can actively control plasmon resonance frequency and amplitude. The hybrids of graphene and metal are used to support the electrostatic gating of localized surface plasmons to achieve reconfigurable optical responses which could be used in adaptive sensors. Similarly,

heterostructures consisting of TMDC interface excitonic transitions with plasmonic modes, which form hybridized states that allow high light absorption and energy funneling at nanointerfaces (Al-Ani *et al.*, 2022). Quantum-dot plasmonic composites Individual electronic levels of quantum dots are employed as reservoirs of charges that interact with metallic plasmons in a deterministic way in which the emission spectra and the energy transfer pathways are determinable. They are hybrid systems that are composed of the quantum tuneability of 2D materials and the field enhancement of plasmonic nanostructures, which offer platforms in order to tune photochemical and optoelectronic processes.

5.5. Device Integration and Quantum Sensing Frontiers

Quantum-plasmonic hybrids are the future of quantum-enabled sensing and catalysis that involves the implementation of quantum-plasmonic hybrids in real devices. The developments of nanofabrication and photonic integration have allowed hybrid components to be incorporated into the on-chip architecture of optical waveguides and resonators that have direct access to quantum-plasmonic active sites. This form of integration allows near field enhancement and photon electron correlation to be applied to detect single molecules, and this technology puts the ultimate limit to sensitivity of detection to the quantum noise limit. In catalysis, the catalysis reaction can be localized by its incorporation of plasmonic nanocavities and quantum emitters via integrated photonic chips to enable reaction specific activation at the lowest possible energy requirements. The same physical principles can be applied to quantum communication and quantum computation, in which hybrid plasmonic elements between photons and solid-state qubits are to be taken as coherent transducers (Lee *et al.*, 2021). The stability of interfaces, scaling decoherence and scalable fabrication of large areas remain critical issues to face, although nanolithography and self-assembled patterning have continued to bridge the gap between nanoscale and scaled quantum technologies.

6. Circular and Sustainable Hybrid Nanomaterials, Engineering for Environmental and Energy Resilience

Circular nanotechnology is a paradigm according to which hybrid nanomaterials are considered as lasting, sustainable, and responsible options to transient and high-performance apparatus in the world. To realize environmental resilience and energy equity, researchers are rearranging the contribution made by materials science through the integration of the principles of the circular economy in the synthesis, use, and end-of-life control of nanomaterials. The most appropriate ones are the hybrid nanomaterials containing organic-inorganic, bio-synthetic, or quantum-plasmonic interfaces because they can be applied to the areas of catalytic, sensing and energy storage (Amarnath *et al.*, 2013). It is the challenge to combine functionality and

eco-efficiency, reduce carbon and toxic footprint without necessarily sacrificing performance. This part describes the concepts of the design, production and application of hybrid nanomaterials in a closed loop and low impact model.

6.1. Principles of Circular Nanomaterial Design

The focus of circular nanomaterial design is on recyclability, reusability, and the need of minimum resource extraction, based upon molecular frameworks which can be dissolved or recreated at the end of their lifetime. New recyclable hybrid structures, including covalent organic framework (COF) metals oxides composites or polymer nanocarbon hybrids allow both mechanical and chemical recovery without structural damage. Functional residues can be reused by creating environmentally benign nanocomposites, which contain biodegradable polymers or bio-sourced ligands, which can degrade. In addition, substituting essential or rare materials like platinum, cobalt, or rare-earth dopants with common ones, including Fe, Ni, Cu, or Mo, is resource-circular and geopolitically secure (Gielen *et al.*, 2022). Additionally to this strategy, material purity and recyclability are improved by solvent minimization and green reaction media (e.g. deep eutectic solvents, supercritical CO₂). These design concepts set a baseline of hybrid nanomaterials that have the ability to circulate unlimited within the production ecosystem similar to the biological process of regeneration.

6.2. Low-Energy and Green Synthesis Strategies

The realization of sustainability starts at the synthetic level, where renewable-feedstock-based, low-energy, and solvent-free processes are quickly replacing the energy intensive processes. Mechanochemical synthesis, which relies on the shear and impact forces, allows solid-state reactions without solvents, significantly decreasing the waste and time of reaction. Microwave-assisted synthesis improves the reaction dynamics by heating the volumetric reaction which facilitates phase uniformity and crystallinity with a low energy input. Similarly, the morphology and oxidation state of electrochemical and photochemical fabrication pathways can be tuned, with renewable electricity or solar photons driving the process. Additional reduction of carbon intensity is achieved by integrating the feedstocks of CO₂, biomass precursors, and stream of waste valorizations (Joarder *et al.*, 2025). As one example, biogenic metal-organic structures based on amino acids or lignin show similar catalytic and adsorption activities compared to traditional systems and are biodegradable. Together these strategies form a green synthesis paradigm, in which the hybrid nanomaterials are produced with insignificant waste, insignificant emissions and high energy consumption.

6.3. Hybrid Nanomaterials in Energy Conversion and Storage

The hybrid nanomaterials have played major roles in the technology of renewable energy conversion

and storage devices and this is because they have the capacity of enabling crossflow of electrons and ions, through establishment of synergies and interfaces in engineering. Semiconductor and conductive metal or carbon network heterojunction catalysts exploit the charge separation maximally and reduce the overpotential of important electrochemical reactions, including CO₂ reduction (CO₂ RR), oxygen evolution (OER) and hydrogen evolution (HER). Photoelectrocatalytic systems. Light-induced charge carriers of plasmonic semiconductor hybrids that enable photoelectrocatalytic systems with a fivefold catalyzing rate compared to conventional catalysts. Hybrid electrodes with 2D materials, metal-organic structures, and conductive polymers can be utilized in the energy storage sector that possesses a higher capacity retention rate performance, particularly in metal-air and solid-state batteries (Liu *et al.*, 2021). Such an architecture balances power density and stability, as well as long-cycle and high-power applications. Combining the sustainable synthesis with high energy efficiency, these materials bring nanotechnology together with the international decarbonization objectives.

6.4. Environmental Remediation and Resource Recovery

Sustainability is not limited to the production process but also to remediation and/or circular recovery, where hybrid nanomaterials can serve as multifunctional pollutants degradation agents, detoxification agents, and elemental recovery agents. Hybrids Photocatalytic hybrids incorporate plasmonic/carbon components to enhance visible light activity and include TiO₂, g-C₃N₄, or ZnO which is shown to be more active in aqueous systems against persistent organic pollutants and pathogens. Hybrid membranes with nanofillers (MOFs or graphene analogs) can be selective in the movement of ions and contaminants as well as resist fouling and degradation. In addition to remediation, nanocatalytic recovery systems also allow extracting useful metals (Au, Pd, Li) in the form of electronic or industrial waste via redox-mediated reactions, which contributes to the material circle (Singh *et al.*, 2025). The applications will make nanomaterials a dual-function system remedier and regenerator that simultaneously clears the environment and reclaims important resources and completes the material lifecycle.

6.5. Policy, Standardization, and Lifecycle Analysis

Incorporating sustainability into nanomaterial science needs to be more than technical achievement and it should also encompass agreement between the regulatory systems and quantifiable eco-metrics. Lifecycle assessment (LCA) models provide an in-depth study of environmental impact in the synthesis, operation, and disposition phases and are applied to streamline the effectiveness of the processes and its recyclability. Eco-design standards such as the ISO 14040 and the EU REACH standards are now being down-scaled to nanoscale materials to ensure that they

are transparent on the issues of toxicity, persistence, and recyclability. The scalability of the industry at the level of green nanomanufacturing principles is soon to be determined through the introduction of safety-by-design, energy audit procedures, and circular performance indicators (Furxhi *et al.*, 2022). Socioeconomic scan indicates that sustainable hybrid nanomaterials can simultaneously enable a state of resource equity, decentralized energy production and low-carbon industrial changes particularly in the emerging economies. This can be achieved by bridging the policy, science and industry with standardized circular structures and hence determine the effectiveness of the hybrid nanotechnologies to planetary sustainability.

CONCLUSION

The next-generation hybrid nanomaterials are the interface between chemistry, physics and engineering whereby it is possible to use multifunctional systems as opposed to the former materials in the sense of sensing accuracy and catalytic efficacies. This can be explained by their functionality, which is due to rational design of interfaces, where the interaction between the electronics and structural and quantum interactions give synergistic behavior. The discovery to predictive design as opposed to trial and error has been revolutionized in the recent developments of machine learning, in situ spectroscopy and self-assembly. Scalable fabrication pathways, which are informed by bioinspiration principles and green chemistry, urgently need to be developed in the future in order to bring the laboratory innovation to practice. The use of digital tools and independent synthesis along with the lifecycle assessment will accelerate the efficiency and environmental suitability. Lastly, hybrid nanomaterials are the future of intelligent, adaptive and responsible material systems and is a new platform of performance to sustainable sensors, energy technologies and catalytic processes that optimizes a sustainable balance between performance and planetary stewardship.

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