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Research Article

# Advances in Nanomaterials for Chemistry-Based Sustainable Energy Technologies: Design Strategies, Performance and Environmental Considerations: Review Article

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**Abstract**

Nanomaterials occupy a pivotal position at the intersection of chemistry and sustainable energy, offering tuneable physicochemical properties that can be leveraged to overcome longstanding efficiency and stability barriers in solar energy conversion, electrochemical storage, and photocatalytic fuel production. This review critically examines recent advances (2020–2025) in the design, synthesis, and performance of key nanomaterial families, including metal oxide nanoparticles, carbon nanotubes, graphene derivatives, MXenes, quantum dots, and perovskite nanocrystals, applied to photovoltaics, supercapacitors, lithium-ion batteries, dye-sensitised solar cells (DSSCs), and photocatalytic hydrogen evolution. We systematically evaluate design strategies encompassing heterojunction engineering, surface passivation, plasmonic enhancement, nanocomposite hybridisation, and green synthesis routes. Performance benchmarks demonstrate power conversion efficiencies exceeding 27% in single-junction perovskite solar cells and specific capacitances surpassing 800 F $g^{-1}$ in MXene-based supercapacitors. Crucially, we address the environmental footprint of these technologies, encompassing ecotoxicological profiles, lifecycle considerations, and safer-by-design principles aligned with global sustainability mandates. Regulatory gaps, scalability challenges, and future research directions integrating machine learning-assisted nanomaterial design are identified. This review serves as a comprehensive resource for chemists, materials scientists, and energy engineers advancing the transition to a low-carbon energy paradigm.

**Keywords:** *nanomaterials; sustainable energy; perovskite solar cells; MXene supercapacitors; photocatalysis; ecotoxicology; green synthesis*

## 1. Introduction

The global energy landscape is under unprecedented pressure to transition away from fossil fuels towards clean, sustainable alternatives. The International Energy Agency (IEA) projects that renewable energy technologies must account for over 80% of global electricity generation by 2050 to limit warming to 1.5 °C above pre-industrial levels. Central to this transition are advances in solar photovoltaics (PV), electrochemical energy storage (EES), and green hydrogen

production via photocatalysis, three domains in which nanomaterials have demonstrated transformative potential.

Nanomaterials, defined by the US National Nanotechnology Initiative as materials with at least one dimension between 1 and 100 nm, exhibit size-dependent properties that diverge dramatically from their bulk counterparts [1]. Quantum confinement effects, exceptional surface-area-to-volume ratios, enhanced charge carrier mobility, and tunable optical band gaps collectively endow these materials with performance characteristics unobtainable at the macroscale. For instance, titanium dioxide (TiO2) nanoparticles exhibit photocatalytic activity several orders of magnitude greater than bulk TiO2, owing to suppressed recombination kinetics and increased reactive surface area [2].

The chemistry underpinning nanomaterial-energy interactions is rich and multifaceted. Heterojunction engineering exploits band alignment at nanoscale interfaces to drive directional charge transfer; plasmonic nanostructures harvest sub-bandgap photons through localised surface plasmon resonance (LSPR); and two-dimensional (2D) materials such as MXenes provide metallic conductivity coupled with redox-active surfaces suitable for pseudocapacitive energy storage [3,4]. These chemical design principles underpin the rapid improvement of device performance metrics reported across the literature in recent years.

Despite considerable promise, the translation of laboratory-scale nanomaterial innovations into commercially viable energy technologies is impeded by challenges including poor long-term stability, high production costs, limited scalability of synthesis methods, and, critically, inadequate understanding of the environmental fate and toxicity of engineered nanomaterials (ENMs) [5,6]. The ecotoxicological profiles of common nanomaterials, from lead-based perovskites to silver nanoparticles, raise legitimate concerns that must be addressed alongside performance optimisation to ensure truly sustainable energy solutions.

This review provides a critical and comprehensive appraisal of the state-of-the-art in nanomaterials for chemistry-based sustainable energy applications, published primarily between 2020 and 2025. Following an overview of nanomaterial classification and synthesis strategies, we examine performance advances in the key application domains of photovoltaics, electrochemical storage, and photocatalytic fuel production. A dedicated section addresses environmental considerations, encompassing ecotoxicology, lifecycle analysis (LCA), and regulatory frameworks. The review concludes with a forward-looking perspective on machine learning-guided design and the critical path towards commercialisation.

## 2. Classification Of Energy-Relevant Nanomaterials

### *2.1 Zero-Dimensional Nanomaterials*

Quantum dots (QDs) are semiconductor nanocrystals typically 2–10 nm in diameter whose optical absorption and emission properties are tunable via the quantum confinement effect by adjusting particle size and composition. Cadmium selenide (CdSe), lead sulfide (PbS), and indium phosphide (InP) QDs have been extensively investigated for photovoltaic applications, with multi-exciton generation (MEG) offering the theoretical possibility of exceeding the Shockley-Queisser efficiency limit [7]. QD solar cells have achieved certified power conversion efficiencies (PCEs) of 20.40%, representing a substantial improvement from the 3% reported in the early 2010s [8].

Metal nanoparticles (NPs), particularly gold, silver, and platinum, serve dual roles as plasmonic antennae and electrocatalytic active sites. In dye-sensitised solar cells (DSSCs), Au NPs embedded within the photoanode exploit LSPR to enhance light absorption in the visible spectrum by 30–50%, while Pt NPs remain the benchmark counter-electrode catalyst, despite their high cost and scarcity [9].

### *2.2 One-Dimensional Nanomaterials*

Carbon nanotubes (CNTs), comprising single-walled (SWCNTs) and multi-walled (MWCNTs) varieties, possess exceptional mechanical strength (Young's modulus ~1 TPa), electrical conductivities exceeding $10^6$ S $m^{-1}$, and large specific surface areas up to 1500 $m^2$ $g^{-1}$ [10]. These attributes make CNTs ideal electrode materials for electrochemical double-layer capacitors (EDLCs), where Boyea et al. demonstrated capacitance and power density improvements over conventional activated carbon through superior conductivity and corrosion resistance [7]. CNTs are also deployed as conductive additives in lithium-ion battery (LIB) electrodes to improve rate capability and cycle life.

### *2.3 Two-Dimensional Nanomaterials*

Graphene and its derivatives, reduced graphene oxide (rGO) and nitrogen-doped graphene, have garnered enormous attention in energy applications owing to their extraordinary in-plane electrical conductivity (~$10^8$ S $m^{-1}$), large theoretical surface area (2630 $m^2$ $g^{-1}$), and chemical versatility [7]. In LIBs, graphene-based anodes accommodate volume expansion during lithiation, while in DSSCs, graphene films function as transparent, flexible counter electrodes displacing expensive platinum.

MXenes, a family of 2D transition metal carbides, nitrides, and carbonitrides derived by selective etching of MAX phases, have emerged as one of the most exciting material classes for energy storage [11]. Ti3C2Tx, the most studied MXene, combines metallic conductivity (~6000 S $cm^{-1}$) with abundant surface terminations (–OH, –O, –F) that support

rapid pseudo-capacitive charge storage [12]. N-doped Ti3C2Tx has demonstrated specific capacitance of 193 F $g^{-1}$ at 2 mV $s^{-1}$ and energy density of 26.22 Wh $kg^{-1}$ over 25,000 cycles in an asymmetric configuration [12].

### *2.4 Three-Dimensional and Hybrid Nanostructures*

Three-dimensional hierarchical nanoarchitectures integrate multiple morphological elements, nanotubes, nanosheets, and nanoparticles into cohesive frameworks that simultaneously optimise light trapping, mass transport, and charge extraction [13]. Perovskite nanocrystals (ABX3, where X = halide) represent a particularly impactful 3D-structured class; their tunable band gaps, high absorption coefficients (>$10^5$ $cm^{-1}$), and long carrier diffusion lengths have propelled PSC efficiencies from 3.8% in 2009 to a certified 27.3% in single-junction configurations by 2025 [14,15]. Table 1 presents the Classification of key nanomaterials, their representative examples, energy applications, and key performance metrics (2020–2025).

**Table 1. Classification of key nanomaterials, their representative examples, energy applications, and key performance metrics (2020–2025).**

| Nanomaterial Type | Representative Examples | Energy Application | Key Performance Metric | Reference |
|---|---|---|---|---|
| Metal oxide NPs | TiO2, ZnO, Fe2O3 | Photocatalytic H2 production | H2 yield: 2150 µmol $g^{-1}$ $h^{-1}$ | [12,13] |
| Carbon nanotubes (CNTs) | SWCNTs, MWCNTs | Supercapacitor electrodes | Capacitance: 404 F $g^{-1}$ | [7,8] |
| Graphene & derivatives | rGO, GO, N-graphene | LIB anodes, solar cells | Specific capacity: 660 F $g^{-1}$ | [8,17] |
| MXenes (2D carbides/nitrides) | Ti3C2Tx, V2CTx, Nb2CTx | Supercapacitors, Li-ion batteries | Csp: 193–570 F $g^{-1}$ | [18,19] |
| Quantum dots (QDs) | CdSe, PbS, CsPbBr3 | Photovoltaics (QDSCs) | PCE: 20.40% | [14,15] |
| Perovskite nanocrystals | MAPbI3, CsPbI3, FASnI3 | Solar cells (PSCs) | PCE: >27% (single-junction) | [14,15,16] |
| Metal nanoparticles | Au, Ag, Pt, Pd NPs | Plasmonic solar cells, fuel cells | Light absorption boost: 30–50% | [14,21] |

## 3. Design Strategies for High-Performance Nanomaterial Energy Devices

### *3.1 Heterojunction and Interface Engineering*

Charge carrier recombination is the primary efficiency-limiting mechanism in both photovoltaic and photocatalytic devices. Heterojunction engineering, the deliberate coupling of two or more semiconductors with staggered band alignments, promotes spatial separation of photogenerated electrons and holes [13]. Type II heterojunctions direct electrons to the material with the lower conduction band minimum and holes to that with the higher valence band maximum, while Z-scheme architectures mimic natural photosynthesis by maintaining high redox potentials in each sub-system. For TiO2-based photocatalysts, coupling with ZnO in a Z-scheme configuration suppresses electron-hole recombination and extends visible-light response, yielding hydrogen evolution rates of 2150 µmol $g^{-1}$ $h^{-1}$ with Pt co-catalyst [13].

In PSCs, interface passivation using self-assembled monolayers (SAMs) and ionic liquids mitigates non-radiative recombination at grain boundaries, contributing to certified PCEs exceeding 25% [14,16]. The electron transport layer (ETL) material choice is equally critical: SnO2 has emerged as a preferred ETL over TiO2 due to its superior band alignment with common perovskite absorbers, wider band gap affording UV stability, and compatibility with low-temperature solution processing [16].

### *3.2 Plasmonic Enhancement Strategies*

Plasmonic nanomaterials absorb electromagnetic radiation through the collective oscillation of conduction electrons, the LSPR effect, generating intense near-field enhancements and hot electrons transferable to adjacent semiconductors [9]. Au NPs incorporated into the photoactive layer or at the perovskite/charge transport layer interface enhance light absorption in the Vis-NIR region and facilitate charge collection, yielding PCE improvements of up to 15% relative to plasmonic-free controls [14]. In TiO2-based photocatalysts, Ag NP decoration lowers the charge carrier recombination rate and shifts the photoresponse into the visible spectrum, enabling solar-driven hydrogen production under AM 1.5G illumination [13].

### *3.3 Nanocomposite Hybridisation*

Combining chemically distinct nanomaterials into composites frequently delivers synergistic performance improvements unattainable by individual components. MXene/carbon hybrid composites illustrate this principle compellingly: CNT-wrapped MXene electrodes exhibit higher capacitance (404 F $g^{-1}$ at 4 A $g^{-1}$) than either material alone, attributable to expanded interlayer spacing facilitating ion transport and CNT-mediated electron highways [18]. Similarly, MXene/rGO composite electrodes deliver 660 F $g^{-1}$ at 0.5 A $g^{-1}$ with 10,000-cycle stability [19]. In DSSCs, polyaniline-CNT composites as counter electrodes outperform pure polyaniline by 30–50% in catalytic activity [9].

### *3.4 Green and Sustainable Synthesis*

Conventional nanomaterial synthesis often employs toxic precursors, corrosive etchants, and energy-intensive processes, undermining the sustainability credentials of the resulting energy devices. Green synthesis routes, including plant extract-mediated bioreduction, microwave-assisted synthesis, and hydrothermal processing using non-hazardous solvents, offer environmentally benign alternatives with comparable or superior product quality [3,13]. For DSSCs, bio-derived sensitisers and natural dye extracts reduce the reliance on synthetic ruthenium complexes, improving ecological compatibility [3]. In MXene synthesis, HF-free etching protocols using fluoride salt/acid combinations are increasingly adopted to reduce occupational and environmental hazards [12]. Table 2 gives the Summary of key design strategies, mechanistic rationale, nanomaterial systems employed, and performance outcomes, while Figure 1 shows the Schematic illustration of major nanomaterial design strategies for sustainable energy devices, including heterojunction charge transfer pathways, plasmonic LSPR enhancement, MXene interlayer engineering, and nanocomposite hybridisation.

**Table 2. Summary of key design strategies, mechanistic rationale, nanomaterial systems employed, and performance outcomes.**

| Design Strategy | Mechanism / Approach | Nanomaterial System | Outcome / Reference |
|---|---|---|---|
| Heterojunction engineering | Type II / Z-scheme charge transfer to reduce recombination | TiO2/ZnO, g-C3N4/TiO2 composites | Enhanced H2 production; [12,13] |
| Surface passivation/doping | Introduce dopant atoms to tailor band gap and defect density | N-doped TiO2, Pb-free perovskites | Improved stability & PCE >25%; [14,16] |
| Nanocomposite hybridisation | Combine 2D materials to synergise conductivity & surface area | MXene/rGO, CNT/graphene hybrids | Csp up to 816 F $g^{-1}$; [18,19,20] |
| Plasmonic enhancement | Localised surface plasmon resonance (LSPR) to boost light absorption | Au NPs on TiO2, Ag/AgBr composites | Visible-light photocatalysis; [13,21] |
| Interface / interlayer engineering | Expand d-spacing for faster ion diffusion; functionalise surface groups | Ti3C2Tx MXene with HMT intercalation | 193 F $g^{-1}$; 25,000 cycle stability; [18] |
| Green / bioinspired synthesis | Plant extract-mediated or low-temperature routes to reduce chemical waste | Green TiO2 NPs, bio-nano DSSC materials | Sustainable fabrication; [3,13] |

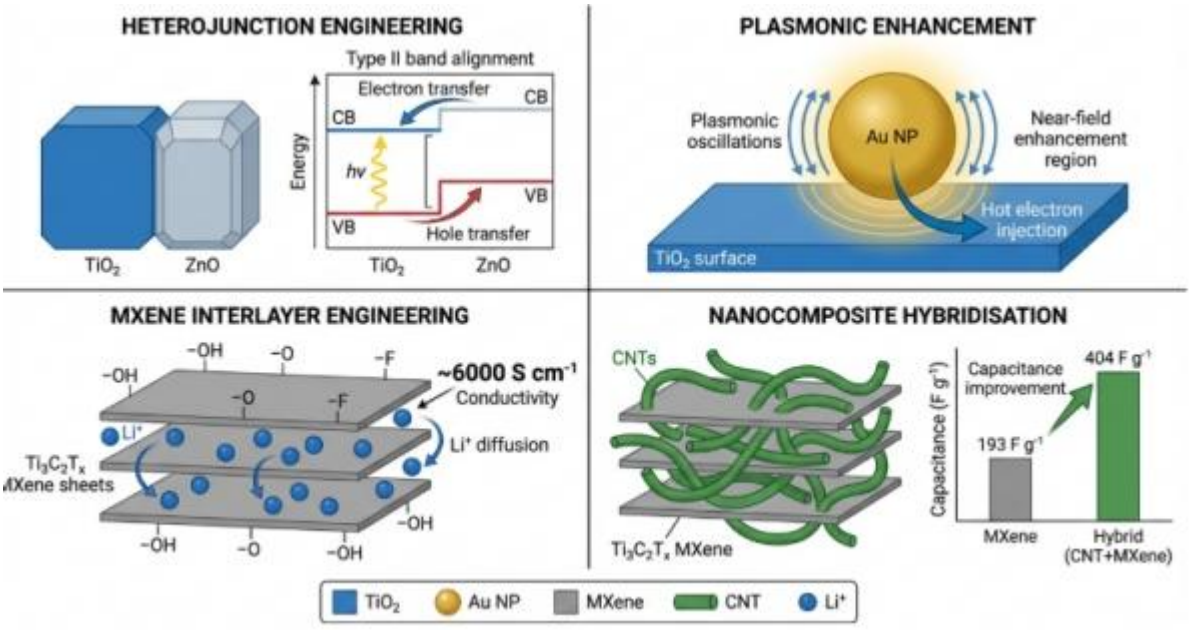


**Figure 1: Schematic illustration of major nanomaterial design strategies for sustainable energy devices, including heterojunction charge transfer pathways, plasmonic LSPR enhancement, MXene interlayer engineering, and nanocomposite hybridisation.**

*Caption: A scientific schematic illustration with a white background divided into four labelled quadrants, each illustrating a distinct nanomaterial design strategy for sustainable energy. Top-left: 'Heterojunction Engineering'- shows a Type II band diagram with two adjacent semiconductor nanostructures (e.g., TiO2 and ZnO), energy level arrows indicating electron transfer to the lower conduction band and hole transfer to the higher valence band, with photon absorption indicated. Top-right: 'Plasmonic Enhancement' - depict a gold nanoparticle on a TiO2 surface with oscillating surface plasmons shown as wave arrows, near-field enhancement highlighted, and hot electron injection indicated by a curved arrow. Bottom-left: 'MXene Interlayer Engineering' - shows layered Ti3C2Tx sheets with surface –OH/–O/–F terminations labelled, intercalated ions (Li+) between layers with blue arrows showing diffusion, and a conductivity value of ~6000 S cm$^{-1}$ annotated. Bottom-right: 'Nanocomposite Hybridisation' - illustrates CNT-wrapped MXene sheets with a capacitance bar showing improvement from 193 to 404 F g$^{-1}$. Use a consistent colour palette (blue for TiO2, gold for Au NPs, grey for MXene, green for CNTs).*

**Sources: Adapted with permission from refs [12,13,14,18].**

## 4. Performance Advances in Key Application Domains

### *4.1 Perovskite Solar Cells*

Metal halide PSCs have emerged as the pre-eminent third-generation photovoltaic technology. The certified PCE of single-junction PSCs has surpassed 27%, and silicon/perovskite tandem cells have exceeded 34%, positioning PSCs as credible competitors to commercial silicon PV [15]. The rapid PCE progression is attributable to multi-pronged advances in crystal regulation, interface passivation, and compositional engineering. Cao et al. reviewed strategies for achieving PCE > 25%, highlighting the role of mixed cation/halide perovskite compositions (Cs/FA/MA triple cations) in simultaneously improving crystallinity, phase stability, and charge transport [14].
SnO2 nanoparticle-based ETLs, modified by surface-active agents such as stable-conformation surfactants, have enabled PCEs of 21.31% with enhanced stability by reducing the density of trap states at the SnO2/perovskite interface [16]. Lead-free perovskites incorporating tin ($Sn^{2+}$) and bismuth ($Bi^{3+}$) remain an active area of research aimed at addressing the substantial toxicity concerns associated with Pb-based absorbers, though PCEs remain below 15% for most Pb-free compositions, necessitating continued materials innovation [15].

### *4.2 Dye-Sensitised Solar Cells (DSSCs)*

DSSCs have attracted renewed interest driven by their low-cost fabrication, compatibility with diffuse light conditions, and tunable aesthetics for building-integrated photovoltaics

(BIPV). Bio-nano composite photoanodes incorporating TiO2 nanoparticles sensitised by natural chromophores offer a sustainable manufacturing pathway, achieving a light-capturing rate improvement of over 10% relative to conventional TiO2 films [3]. The key photovoltaic mechanism in DSSCs relies on photon absorption by the sensitiser, electron injection into the TiO2 conduction band, and regeneration of the oxidised dye by the electrolyte redox couple. Optimisation of the TiO2 nanoparticle network morphology, particularly the adoption of hierarchical architectures combining nanoparticles with nanowires or nanotubes, enhances electron transport and reduces back-recombination [3,9].

### *4.3 MXene-Based Supercapacitors*

Supercapacitors bridge the gap between conventional capacitors and batteries, offering high power density, rapid charge–discharge rates, and exceptional cycling stability. MXene-based electrodes have achieved remarkable volumetric capacitances of 244.13 F $cm^{-3}$, outperforming most carbon-based materials, due to the combination of metallic conductivity and pseudocapacitive redox activity at surface termination sites [18]. However, the tendency for MXene sheets to restack limits ion accessibility; this challenge is addressed through three-dimensional aerogel architectures, polymer intercalation, and incorporation of spacer nanomaterials such as GO and CNTs [19,20]. Asymmetric supercapacitor devices employing DAAQ-modified Ti3C2Tx/graphene composites have achieved energy densities of 43 Wh $kg^{-1}$, approaching those of lead-acid batteries [19].

### *4.4 Lithium-Ion Batteries*

Nanostructured electrode materials dramatically improve LIB performance by reducing ion diffusion path lengths, accommodating volume changes during charge-discharge cycles, and providing additional intercalation sites [7]. Silicon-based anodes, with a theoretical capacity of 3579 mAh $g^{-1}$, ten-fold that of graphite, suffer from severe volume expansion (>300%) during lithiation; nanostructuring into particles below 150 nm reduces particle fracture, while carbon coatings maintain electrical connectivity [7]. MXene-based hybrid anodes and separators additionally improve rate capability and suppress lithium dendrite formation, enhancing both energy density and safety [11].

### *4.5 Photocatalytic Hydrogen Production*

Solar-driven water splitting represents the ultimate sustainable energy conversion process, coupling photon absorption with proton reduction to generate clean hydrogen fuel. TiO2 remains the archetype photocatalyst owing to its chemical stability, non-toxicity, and abundance, but its wide band gap (3.2 eV, anatase) restricts solar light utilisation to the UV region (~4% of the solar spectrum) [13]. Strategies to overcome this limitation include non-metal doping (N, S, C) to introduce intraband gap states, heterojunction formation with narrow band gap semiconductors, and plasmonic sensitisation with noble metal NPs [21]. Advanced TiO2 photocatalytic systems employing Au–TiO2 nanocomposites have achieved dual-function dye degradation and hydrogen production under visible light, with photocurrent densities improved through the unique architecture of Cu-doped TiO2 nanowire films [13,21]. Figure 2 Shows (a) Timeline of certified power conversion efficiency (PCE) progression in single-junction perovskite solar cells from 2020 to 2025, showing key milestones above 25%. (b) Comparative bar chart of specific capacitance values reported for MXene-based supercapacitor electrode configurations

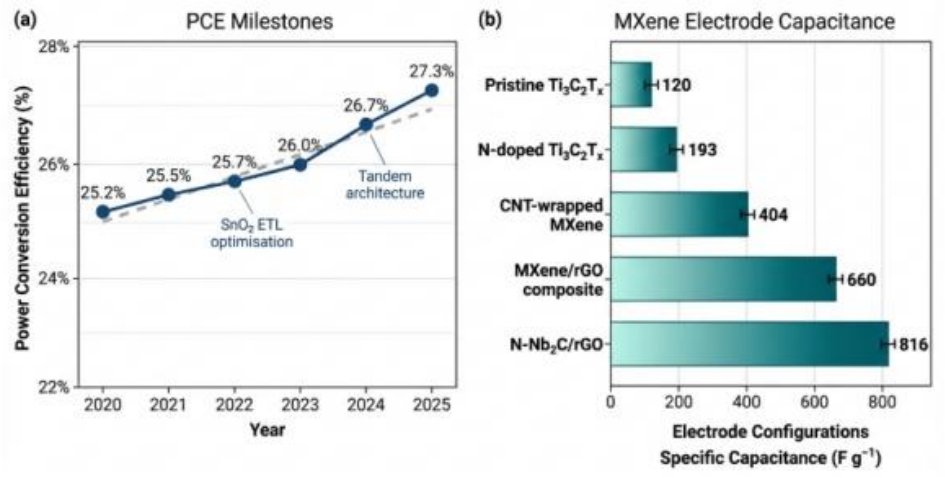


**Figure 2: Shows (a) Timeline of certified power conversion efficiency (PCE) progression in single-junction perovskite solar cells from 2020 to 2025, showing key milestones above 25%. (b) Comparative bar chart of specific capacitance values reported for MXene-based supercapacitor electrode configurations.**

*Caption: A two-panel scientific figure (panel a and panel b) with a clean white background suitable for publication. Panel (a): A line graph with timeline on the x-axis (2020 to 2025) and Power Conversion Efficiency (PCE, %) on the y-axis (ranging from 22% to 28%). Plot PCE milestones as filled circle data points connected by a dashed trend line: 2020: 25.2%, 2021: 25.5%, 2022: 25.7%, 2023: 26.0%, 2024: 26.7%, 2025: 27.3%. (b): A grouped horizontal bar chart comparing specific capacitance (F $g^{-1}$) for five MXene-based electrode configurations: (1) Pristine Ti3C2Tx: 120 F $g^{-1}$, (2) N-doped Ti3C2Tx: 193 F $g^{-1}$, (3) CNT-wrapped MXene: 404 F $g^{-1}$, (4) MXene/rGO composite: 660 F $g^{-1}$, (5) N-Nb2C/rGO: 816 F $g^{-1}$.*

**Source: Data compiled from refs [14,15,18,19].**

## 5. Environmental Considerations and Safer-By-Design Principles

### *5.1 Ecotoxicological Profiles of Energy Nanomaterials*

The widespread deployment of nanomaterials in energy devices inevitably raises questions about their environmental fate following manufacturing, use-phase leaching, and end-of-life disposal. The manufacturing rate of nano-enabled products has increased dramatically, and contamination of environmental matrices with nanoparticles is considered inevitable [22]. Ecotoxicological risk assessment typically employs species sensitivity distributions (SSDs), comparing predicted environmental concentrations (PECs) with

predicted no-effect concentrations (PNECs) derived from dose-response data across multiple trophic levels.

Silver nanoparticles exhibit the highest aquatic ecotoxicity among commonly used energy nanomaterials, with PNEC values as low as $4.85 \times 10^{-5}$ mg $L^{-1}$, attributable to $Ag^{+}$ ion release and oxidative stress induction [22]. TiO2 NPs, conversely, display a PNEC of 0.192 mg $L^{-1}$, reflecting their lower intrinsic toxicity, though photocatalytically-generated reactive oxygen species (ROS) under UV irradiation can cause oxidative damage to aquatic organisms at higher concentrations [24]. Cadmium-containing QDs pose chronic toxicity risks through $Cd^{2+}$ leaching, particularly in acidic environments, necessitating the transition to Cd-free alternatives [23]. Lead-based perovskites present a significant hazard; water ingress can dissolve $Pb^{2+}$ from unstable perovskite phases, contaminating soil and groundwater, underscoring the urgency of Pb-free perovskite development and robust device encapsulation [22,23].

### *5.2 Environmental Fate and Biomolecular Transformations*

ENMs in the environment undergo complex physicochemical transformations driven by their interaction with natural organic matter (NOM), ions, UV radiation, and biological secretions. The formation of an eco-corona, a dynamic layer of proteins, lipids, and polysaccharides adsorbed onto the nanoparticle surface, fundamentally alters colloidal stability, bioavailability, and toxicity [25]. Sulfidation of Ag NPs in sulfide-rich sediments reduces their toxicity by transforming soluble $Ag^{+}$ to poorly soluble Ag2S, while photo-oxidation of TiO2 NPs in sunlit surface waters generates additional ROS, potentially increasing biological effects. These dynamic transformations must be incorporated into predictive environmental risk assessment models.

### *5.3 Mixture Toxicity and Cumulative Effects*

Energy devices typically contain multiple nanomaterial types in proximity, and their co-release into environmental matrices creates mixture toxicity scenarios that may deviate significantly from predictions based on individual components. Binary mixtures of Cu and ZnO NPs exhibit enhanced (synergistic) toxicity to Oncorhynchus mykiss, while antagonistic effects have been observed for the same combination in different species, reflecting the species- and media-dependent nature of mixture interactions [25]. Comprehensive ecotoxicological testing covering multiple trophic levels, exposure conditions, and NP combinations is therefore essential for credible risk assessment.

### *5.4 Safer-by-Design and Lifecycle Considerations*

The safer-by-design paradigm advocates for the integration of safety and sustainability considerations into the earliest stages of nanomaterial development, rather than as ex post risk mitigation [24]. Key principles include substitution of hazardous constituents (e.g., replacing Pb in PSCs with Sn or Bi; replacing Cd in QDs with Zn or In), surface modification to reduce dissolution and bio-uptake, and design for end-of-life recyclability. Lifecycle assessment (LCA) tools are essential for holistic sustainability evaluation, quantifying energy inputs, material flows, and environmental emissions across the entire product lifecycle from raw material extraction to device disposal [4,5]. Studies on TiO2-based photocatalytic systems indicate that the energy payback period, the time for the device to produce as much energy as consumed in its manufacture, is a critical metric that must be minimised through process optimisation and renewable energy-powered synthesis. Table 3 shows the Environmental concerns, affected ecosystems, and mitigation strategies for nanomaterials commonly deployed in sustainable energy devices, while Figure 3 gives the A Conceptual framework illustrating the environmental lifecycle of energy nanomaterials: from synthesis and device integration, through use-phase leaching and end-of-life release, to environmental fate (eco-corona formation, transformation, bioaccumulation), ecotoxicological endpoints, and safer-by-design feedback loops

**Table 3. Environmental concerns, affected ecosystems, and mitigation strategies for nanomaterials commonly deployed in sustainable energy devices.**

| Nanomaterial | Environmental Concern | Affected Ecosystem | Mitigation Strategy / Reference |
|---|---|---|---|
| Lead-based perovskites (PbI2) | Lead leaching, aquatic toxicity | Aquatic, terrestrial | Pb-free alternatives (Sn, Bi); encapsulation; [22,23] |
| Silver NPs (Ag NPs) | High ecotoxicity (PNEC: $4.85\times10^{-5}$ mg/L); ion release | Aquatic organisms | Stabilising coatings; concentration control; [22,23] |
| TiO2 NPs | ROS generation under UV, photocatalytic oxidative stress | Aquatic biota, soil microbiome | Safe-by-design; surface modification; [22,24] |
| Carbon nanotubes (CNTs) | Biopersistence, pulmonary inflammation risk | Human health, terrestrial | Functionalisation to reduce aspect ratio; [24] |
| MXenes (Ti3C2Tx) | HF used in synthesis; oxidation byproducts | Aquatic, occupational | HF-free etching; in situ passivation; [18,25] |
| Quantum dots (CdSe, PbS) | Cd/Pb toxicity; long-term persistence | Food chain, aquatic | Transition to Cd-free QDs (InP, ZnSe); lifecycle assessment; [23] |

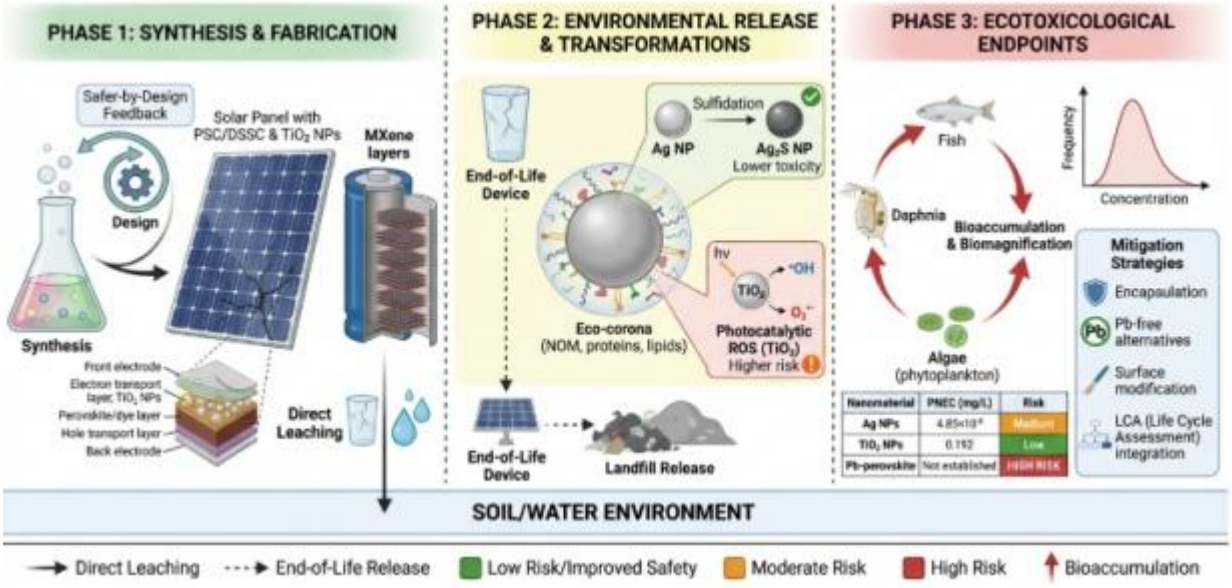


**Figure 3: A Conceptual framework illustrating the environmental lifecycle of energy nanomaterials: from synthesis and device integration, through use-phase leaching and end-of-life release, to environmental fate (eco-corona formation, transformation, bioaccumulation), ecotoxicological endpoints, and safer-by-design feedback loops.**

*Caption: A comprehensive conceptual lifecycle and environmental fate diagram for energy nanomaterials on a white background. The diagram flows from left to right across three main phases separated by vertical dashed lines. Phase 1 (Synthesis & Fabrication, green zone): Shows icons for (a) a chemical/hydrothermal synthesis flask, (b) a solar panel incorporating PSC/DSSC with TiO2 NPs, and (c) a supercapacitor cylinder with MXene layers. Includes a 'Safer-by-Design' circular feedback arrow connecting synthesis back to design choices. Phase 2 (Environmental Release, yellow zone): Show arrows from device to environment representing leaching pathways (solid arrows from cracked solar panel, dashed arrow from landfill). In the centre, illustrate a nanoparticle with an adsorbed layer labelled 'Eco-corona (NOM, proteins, lipids)'. Show environmental transformations: sulfidation of Ag NPs (Ag NPs → Ag2S, lower toxicity), photocatalytic ROS generation from TiO2 NPs (TiO2 + hv → •OH + O2•⁻, higher risk). Phase 3 (Ecotoxicological Endpoints, red zone): Draw a three-trophic-level food chain (algae → daphnia → fish) with ascending bioaccumulation arrows. Includes a mini-SSD (species sensitivity distribution) curve. And a PNEC comparison table beside it showing Ag NPs ($4.85\times10^{-5}$*

*mg/L), TiO2 (0.192 mg/L), Pb-perovskite (HIGH RISK, no PNEC established). At the far right, shows a 'Mitigation Strategies' box shows: encapsulation, Pb-free alternatives, surface modification, LCA integration.*

**Sources: Adapted from concepts in refs [22,23,24,25].**

## 6. Challenges and Future Perspectives

Notwithstanding the remarkable performance advances documented in this review, several critical challenges must be addressed before nanomaterial-based sustainable energy technologies achieve widespread commercial deployment. First, long-term operational stability remains a principal concern for PSCs; while laboratory PCE records are impressive, devices must demonstrate >25-year lifetimes under outdoor conditions (temperature cycling, humidity, UV exposure) comparable to silicon PV. Encapsulation strategies, compositional engineering (Cs-containing multi-cation perovskites), and 2D/3D heterostructure architectures are active research fronts targeting this challenge [15,16].
Second, the scalability of nanomaterial synthesis from gram-scale laboratory batches to industrial production quantities remains a formidable obstacle. Solution-based methods such as hydrothermal synthesis and sol-gel processing offer more scalable routes than vapour deposition techniques, but batch-to-batch reproducibility, cost of high-purity precursors, and energy intensity of processing must all be optimised [4,5]. Third, the environmental and toxicological knowledge base for many emerging nanomaterials, particularly MXenes and halide perovskites, remains insufficient to support robust regulatory decision-making. Accelerated ecotoxicological testing programmes, standardised characterisation protocols, and predictive computational toxicology models are urgently required [22,24].

Looking ahead, machine learning (ML) and artificial intelligence (AI) offer transformative potential for nanomaterial design by enabling high-throughput screening of vast compositional and structural spaces inaccessible to conventional experimental programmes. ML-assisted identification of optimal perovskite compositions, co-catalyst pairings for photocatalysis, and MXene surface terminations for targeted energy storage metrics is an active and rapidly evolving field [15]. Integration of multi-scale computational modelling, from density functional theory (DFT) at the atomic scale to finite element modelling at the device scale, with automated synthesis platforms, will accelerate the translation of computational predictions into experimental validation.

Furthermore, the integration of nanomaterial-based energy devices with emerging digital technologies, including the Internet of Things (IoT), smart grids, and wearable electronics, creates demand for flexible, lightweight, and self-powered systems that exploit the mechanical adaptability of 2D nanomaterials and quantum dot-based sensors. Conductive polymer-nanomaterial composites represent promising electrode materials for flexible supercapacitors and organic photovoltaics in this context [8,9].

## 7. Conclusion

This review has demonstrated that nanomaterials occupy a central and irreplaceable role in advancing chemistry-based sustainable energy technologies. From the certified PCE > 27% of single-junction perovskite solar cells engineered through precision interface chemistry, to MXene supercapacitors delivering 816 F $g^{-1}$ through 2D nanoarchitecture design, and TiO2-based photocatalysts generating hydrogen at 2150 µmol $g^{-1}$ $h^{-1}$ via plasmonic and heterojunction strategies, the performance gains achieved through rational nanomaterial design are substantial and continuing. Equally important is the growing recognition that these technological advances must be accompanied by rigorous environmental stewardship, encompassing ecotoxicological assessment, lifecycle analysis, and safer-by-design integration, to ensure that the transition to sustainable energy does not inadvertently create new environmental burdens. The convergence of advanced synthesis chemistry, computational materials design, and holistic sustainability assessment positions nanomaterials as foundational enablers of the global clean energy transition.

## Author Contributions

The author has significantly contributed to the study's conception, design, data collection, analysis, and interpretation. All authors were involved in writing the manuscript or critically reviewing it for its intellectual value. They have reviewed and approved the final version for submission and publication and accept full responsibility for the content and integrity of the work.

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## Conflicts of Interest

The authors state that there are no financial, personal, or professional conflicts of interest associated with this research.

## Ethical Approvals

This research did not involve the use of human participants or animal subjects and therefore did not require ethical clearance

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