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Interface-programmed nano energy systems for coupled solar conversion and thermoelectric power: a critical mini-review and translational roadmap

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Nano-enabled solar, thermoelectric, and hybrid photovoltaic–thermoelectric (PV–TEG) systems offer promising routes for improving renewable-energy utilization, yet the field remains fragmented across material classes, device architectures, and isolated performance metrics. This PRISMA-guided critical mini-review synthesizes 74 studies on nanomaterials for solar conversion, thermoelectric generation, and hybrid PV–TEG integration. The review develops an interface-programmed nano-energy framework in which photon absorption, charge-carrier extraction, phonon-mediated heat transport, interfacial thermal resistance, and device stability are treated as coupled design variables rather than separate material functions. The synthesis shows that quantum dots, perovskite nanocrystals, plasmonic nanoparticles, nanowires, superlattices, hierarchical nanocomposites, carbon nanomaterials, and two-dimensional materials enhance energy conversion mainly when their interfaces coordinate optical, electronic, and thermal pathways. For hybrid PV–TEG systems, the review shows that simple device stacking is insufficient because practical net energy gain depends on photovoltaic temperature control, thermal contact resistance, preservation of the thermoelectric temperature gradient, electrical load matching, packaging reliability, and comparison with PV-only and TEG-only references under matched operating conditions. The review further identifies a stability–toxicity–scalability trilemma that limits translation of high-efficiency or high-ZT nanomaterials into deployable energy systems, particularly for Pb-, Cd-, Te-, noble-metal-, and heat-sensitive platforms. To improve transparency and comparability, the review proposes an evidence-summary table, descriptive graphical synthesis, semi-quantitative material scoring, and a reporting checklist covering material identity, synthesis route, device architecture, performance metrics, stability testing, toxicity/sustainability evidence, scalability indicators, and net hybrid gain. Overall, this mini-review argues that future progress in nano-energy systems will depend on mechanism-aware, interface-programmed co-design that integrates efficient solar conversion, useful waste-heat recovery, durable interfaces, safer material chemistry, scalable processing, and validated system-level energy benefit.

KEYWORDS
energy conversion, interface engineering, nano energy systems, nanomaterials, photovoltaic–thermoelectric integration

1 Introduction

The global energy transition requires power-generation technologies that are efficient, durable, low-carbon, scalable, and adaptable to both centralized and decentralized energy systems (Shen et al., 2025; Okesiji, 2025; Eze et al., 2024). Solar photovoltaics have emerged as one of the most rapidly expanding renewable energy technologies, while thermoelectric generators offer a solid-state route for converting temperature gradients, industrial waste heat, and device-level heat losses into useful electricity (Bhagat et al., 2025; Anwar et al., 2026). However, both technologies remain constrained by fundamental and translational limitations. Photovoltaic devices lose a substantial fraction of incident solar energy through thermalization, optical reflection, transmission, carrier recombination, resistive losses, and heat dissipation (Saeed and Zohaib, 2022; Shen et al., 2020). Thermoelectric devices, in contrast, are limited by the difficulty of simultaneously achieving a high Seebeck coefficient, high electrical conductivity, and low thermal conductivity within the same material system (Shi et al., 2025; Eze, 2025a). Nanotechnology offers a powerful route for addressing these limitations because nanoscale materials enable selective control of optical, electronic, thermal, and interfacial processes (Mbakaan et al., 2025; Eze et al., 2025a). At reduced dimensions, quantum confinement, high surface-to-volume ratio, interface engineering, defect modulation, and phonon scattering can be exploited to improve light absorption, charge separation, carrier transport, thermal management, and energy conversion efficiency (Nag and Chaudhuri, 2026; Bansal et al., 2026). Consequently, quantum dots, perovskite nanocrystals, plasmonic nanoparticles, nanowires, nanotubes, two-dimensional nanosheets, superlattices, and hierarchical nanocomposites have become central material platforms in next-generation solar and thermoelectric research (Singh A. K. et al., 2025; Baby et al., 2026; Boretti, 2025).

Despite substantial progress, the nano-energy literature remains fragmented. Solar-energy studies frequently emphasize power conversion efficiency, bandgap engineering, light management, and interface passivation. In contrast, thermoelectric studies often focus on figure of merit, phonon scattering, carrier mobility, and thermal conductivity suppression. Hybrid photovoltaic-thermoelectric systems are commonly presented as device-level combinations rather than as fully integrated nano-energy architectures governed by coupled photon, carrier, phonon, and interface dynamics. This separation limits the development of design principles that can translate nanoscale performance gains into stable, scalable, and application-ready energy systems. This review addresses that gap by reframing solar conversion and thermoelectric power generation as a coupled nano-energy problem. It argues that the next major advance will not come merely from discovering additional nanomaterials, but from programming interfaces to regulate energy flow across optical, electrical, thermal, and structural domains. By linking material class, performance mechanism, device architecture, and translational barrier, this review provides a critical framework for interface-programmed nano-energy systems and highlights how hybrid photovoltaic-thermoelectric platforms can be designed for improved energy utilization, durability, and scalability.

1.1 Solar energy conversion, thermal loss pathways, and the rationale for PV-TEG coupling

Solar-energy technologies can be broadly understood as systems that convert incident solar radiation into useful thermal, electrical, or chemical energy. Passive solar-energy systems rely primarily on architectural orientation, material thermal mass, natural lighting, and heat-retention strategies to capture and regulate solar heat without active mechanical or electrical conversion. Active solar-energy systems, in contrast, use engineered devices such as photovoltaic modules, solar thermal collectors, concentrators, photothermal absorbers, photoelectrochemical cells, and hybrid solar-energy harvesters to convert solar radiation into electricity, heat, fuels, or combined energy outputs. Within this broad landscape, photovoltaic technology has become the dominant direct solar-to-electricity pathway because it converts photons into electrical power through semiconductor light absorption, charge-carrier generation, carrier separation, and external current extraction.

In conventional photovoltaic operation, only part of the incident solar spectrum is converted into useful electrical power. Photons with energy below the absorber bandgap are not absorbed efficiently, while photons with energy above the bandgap lose excess energy through carrier thermalization. Additional losses arise from optical reflection, incomplete absorption, transmission, non-radiative recombination, series resistance, shunt pathways, contact losses, spectral mismatch, and module-level parasitic effects (Saeed and Zohaib, 2022; Shen et al., 2020). A substantial fraction of the absorbed solar energy is therefore dissipated as heat. This heat accumulation increases photovoltaic operating temperature, which can reduce open-circuit voltage, lower power conversion efficiency, accelerate material degradation, and intensify encapsulant, contact, and interfacial failure. Thermal management is consequently not a secondary engineering issue, but a central factor governing photovoltaic performance, stability, and lifetime.

Several thermal-management strategies have been explored to mitigate photovoltaic heat losses, including passive heat sinks, phase-change materials, forced air or liquid cooling, photovoltaic-thermal collectors, radiative cooling layers, spectrally selective coatings, photothermal interlayers, and thermal interface materials (Bhagat et al., 2025; Anwar et al., 2026; Kim et al., 2019). These approaches aim either to reduce the photovoltaic operating temperature, recover otherwise wasted heat, or redistribute heat away from temperature-sensitive layers. However, heat removal alone does not necessarily increase total energy utilization unless the extracted thermal energy is converted into useful output or contributes to system-level performance. This creates a strong rationale for waste-heat recovery concepts, particularly in hybrid solar architectures where residual heat can be harvested rather than simply dissipated.

Thermoelectric generators provide one route for converting a temperature gradient directly into electrical power through the Seebeck effect. When coupled to photovoltaic devices, a thermoelectric stage can in principle recover part of the heat generated by thermalization and other loss pathways while the photovoltaic stage continues to produce direct electrical output. Recent PV-TEG studies have explored different coupling strategies,

including monolithic photovoltaic-thermoelectric generators using exothermic reactive interlayers, dye-sensitized solar cell-thermoelectric hybrid generators based on unified bipolar-conduction elements, bandgap-engineered metal-oxide systems, black TiO_2-based photothermal layers, and flexible PIN-type photo-thermoelectric configurations (Kim et al., 2019; Kim et al., 2020; Parkavi et al., 2026; Parkavi et al., 2025; Prabhu et al., 2026). These examples show that PV-TEG integration is not limited to simple physical stacking, but can involve engineered interlayers, absorber modification, photothermal conversion, thermal-gradient control, and flexible device architectures.

However, this coupling is not automatically beneficial. If the thermoelectric module increases the photovoltaic temperature, introduces excessive thermal contact resistance, fails to preserve a sufficient temperature difference across the thermoelectric legs, or adds electrical and packaging losses, the integrated system may perform worse than a photovoltaic-only reference. Therefore, PV-TEG integration must be evaluated by true net system-level gain rather than by the simple addition of photovoltaic and thermoelectric outputs (Kim et al., 2019; Kim et al., 2020; Parkavi et al., 2026; Parkavi et al., 2025; Prabhu et al., 2026).

This context motivates the interface-programmed nano-energy framework developed in this review. At the nanoscale, optical, electronic, thermal, and mechanical interfaces can be engineered to regulate photon absorption, charge-carrier extraction, phonon-mediated heat transport, thermal-gradient preservation, and device stability. Nanostructured absorbers, quantum dots, perovskite nanocrystals, plasmonic nanoparticles, bandgap-engineered metal oxides, black TiO_2 photothermal materials, two-dimensional materials, carbon nanomaterials, superlattices, and hierarchical thermoelectric nanocomposites are, therefore, not only performance-enhancing materials; they are potential interface-control platforms (Nag and Chaudhuri, 2026; Bansal et al., 2026; Singh A. K. et al., 2025; Baby et al., 2026; Boretti, 2025; Kim et al., 2019; Kim et al., 2020; Parkavi et al., 2026; Parkavi et al., 2025; Prabhu et al., 2026). The central challenge is to design coupled solar-thermoelectric architectures in which photon, carrier, phonon, and heat-flow pathways cooperate rather than compete. This review consequently focuses on nano-enabled solar conversion, thermoelectric generation, hybrid PV-TEG integration, and the translational requirements needed to convert laboratory-scale performance into stable, scalable, and environmentally responsible energy systems.

1.2 Knowledge gap, novelty, and contribution of this review

Although nano-enabled solar conversion and thermoelectric power generation have been widely reviewed, much of the existing literature remains organized around isolated material classes, single-device performance metrics, or separate energy-conversion mechanisms. Solar-focused reviews commonly emphasize absorber engineering, bandgap tuning, defect passivation, light management, and power conversion efficiency. Thermoelectric reviews, in contrast, often focus on the figure of merit, phonon scattering, carrier mobility, and lattice thermal conductivity reduction. Hybrid photovoltaic–thermoelectric systems are frequently discussed as device combinations rather than as integrated nano-energy architectures governed by coupled photon, carrier, phonon, and interfacial heat-flow processes.

This separation creates an important knowledge gap because the performance of hybrid nano-energy systems depends not only on the intrinsic properties of individual materials, but also on how interfaces regulate light absorption, charge extraction, heat localization, thermal-gradient preservation, and mechanical compatibility. To make the interface-programmed framework practically actionable, these interfacial functions should be linked to measurable design criteria rather than treated only descriptively. In hybrid PV–TEG systems, the photovoltaic rear interface, thermal interface material, thermoelectric hot side, cold-side heat sink, and electrical interconnects should be evaluated using area-specific interfacial thermal resistance, heat-transfer efficiency, temperature drop across passive contact layers, temperature difference across the thermoelectric legs, electrical contact resistance, and net hybrid power gain. As a practical screening guide, the area-specific thermal resistance of the PV–TEG thermal contact should preferably be kept in the order of 10–6–10–4 m^2 K W–1, depending on device architecture, contact pressure, bond-line thickness, and mechanical compliance. For thermoelectric operation, contact losses should also be limited relative to the intrinsic leg resistance; thermal contact resistance should ideally contribute less than about 20% of the total leg thermal resistance, while electrical contact resistance should remain below about 30% of the leg electrical resistance to avoid severe efficiency penalties. Therefore, an interface-programmed PV–TEG system should be considered practically effective only when it maintains or lowers photovoltaic operating temperature, preserves a useful temperature gradient across the TEG, minimizes thermal and electrical contact losses, and demonstrates positive net system-level power gain compared with PV-only and TEG-only references tested under identical illumination, ambient temperature, heat-sink condition, device area, and load-matching conditions (Bjørk, 2015; Park et al., 2015; Huxtable et al., 2003).

This review addresses that gap by proposing an interface-programmed nano-energy framework in which solar conversion and thermoelectric generation are treated as coupled processes. The framework links four interacting pathways: photon management, charge-carrier transport, phonon-mediated heat flow, and interfacial thermal regulation. This approach allows nanomaterials such as quantum dots, perovskite nanocrystals, plasmonic nanoparticles, superlattices, hierarchical nanocomposites, and two-dimensional materials to be evaluated not only by their reported performance but also by their mechanistic role and translational feasibility.

This mini-review makes four specific contributions. First, it reframes nano-enabled solar and thermoelectric systems as integrated photon–carrier–phonon–interface architectures rather than independent device platforms. Second, it introduces the stability–toxicity–scalability trilemma as a practical lens for assessing whether high-performing nanomaterials can realistically progress toward deployment. Third, it maps representative nanomaterial classes to their dominant mechanisms, device opportunities, and translational barriers. Fourth, it proposes a reporting and benchmarking checklist to improve reproducibility, comparability, and application relevance in future nano-energy studies.

This repositioning is important because descriptive reviews alone are no longer sufficient for a rapidly expanding field. A translational relevance review must move beyond listing nanomaterials and instead explain how nanoscale mechanisms can be coordinated into stable, scalable, and environmentally acceptable energy systems. The central argument of this review is therefore that the next major advance in nano-energy research will depend on interface-programmed co-design, where optical, electronic, thermal, and structural functions are integrated within one translationally viable architecture.

However, this review also adopts a critical and balanced position. Although nanostructured absorbers, quantum dots, perovskite nanocrystals, plasmonic nanoparticles, superlattices, hierarchical thermoelectric nanocomposites, carbon nanomaterials, and two-dimensional materials have produced important advances in solar conversion, thermoelectric generation, and hybrid PV–TEG systems, the current evidence base remains uneven. Many studies emphasize peak photovoltaic efficiency, enhanced light absorption, improved power factor, high ZT, or additional thermoelectric output, but provide limited evidence on long-term operational stability, toxicity/safety, reproducibility, scalable fabrication, contact durability, heat-sink dependence, module-level performance, and true net system-level gain. In solar nanomaterials, apparent performance improvements may be offset by trap-state formation, ligand-limited carrier transport, ion migration, heavy-metal toxicity, moisture sensitivity, or poor large-area uniformity. In thermoelectric nanostructures, reduced lattice thermal conductivity may be accompanied by carrier-mobility loss, brittle interfaces, phase segregation, contact resistance, or thermal-cycling fatigue. In hybrid PV–TEG systems, reported output enhancement may reflect additive device reporting rather than genuine net energy gain under matched PV-only, TEG-only, and integrated operating conditions. Therefore, this review does not only summarize promising nano-energy platforms; it critically evaluates whether reported mechanisms are supported by stability, safety, scalability, and device-level evidence.

2 Methods

2.1 Review design

This study adopted a PRISMA-guided systematized critical mini-review design to synthesize evidence on nanoscale materials, nanoscale interfaces, solar conversion, thermoelectric power generation, and hybrid photovoltaic–thermoelectric (PV–TEG) systems. The review was designed as a focused critical synthesis rather than a quantitative meta-analysis because the included literature spans heterogeneous material classes, device architectures, operating temperatures, stability protocols, and performance metrics. PRISMA principles were applied to improve transparency in article identification, screening, eligibility assessment, and inclusion. The purpose was not to exhaustively map every publication in nano-energy research, but to identify representative and mechanistically relevant studies that explain how nanomaterials regulate photon absorption, charge-carrier transport, phonon-mediated heat flow, interfacial thermal resistance, stability, toxicity, and scalability.

2.2 Literature search strategy

A structured literature search was conducted across databases relevant to materials science, energy conversion, nanotechnology, chemistry, engineering, and safety assessment as shown in Table 1. The databases consulted were Scopus, Web of Science, ScienceDirect, PubMed, IEEE Xplore, ACS Publications, RSC Publishing, SpringerLink, and Google Scholar. These sources were selected to capture literature on photovoltaic nanomaterials, thermoelectric nanostructures, PV–TEG systems, quantum dots, perovskite nanocrystals, plasmonic materials, nanocomposites, two-dimensional materials, device integration, and translational barriers. Search terms were combined using Boolean operators. Representative keywords included nano energy, nanostructuring, quantum dots, perovskite nanocrystals, plasmonics, superlattices, nanocomposites, two-dimensional materials, photovoltaics, photoelectrochemical conversion, thermoelectrics, waste heat recovery, PV–TEG, stability, toxicity, scalability, and interface engineering.

A representative Boolean string was used (nano OR nanostructure OR “quantum dot” OR “perovskite nanocrystal” OR plasmonic OR superlattice OR nanocomposite OR “two-dimensional material”) AND (“solar conversion” OR photovoltaic OR photoelectrochemical OR thermoelectric OR “waste heat” OR “photovoltaic-thermoelectric” OR PV–TEG) AND (efficiency OR ZT OR stability OR scalability OR interface). The search focused primarily on studies published between 2020 and 2026, while earlier foundational papers were retained where necessary to explain theoretical principles, historical development, or landmark mechanisms. The final database search was completed on 25 April 2026. Only English-language publications were considered. Eligible sources included experimental studies, computational studies, high-quality review articles, and foundational studies directly relevant to nano-enabled solar conversion, thermoelectric generation, or hybrid PV–TEG systems. The final evidence pool consisted of 74 studies used for synthesis.

2.3 Eligibility criteria

Explicit inclusion and exclusion criteria were applied to maintain relevance, methodological clarity, and thematic coherence.

2.3.1 Inclusion criteria

Studies were included if they met at least one of the following conditions: they addressed nanoscale materials, nanostructured interfaces, or nano-enabled device architectures in solar conversion, thermoelectric power generation, or hybrid PV–TEG systems; reported material design, synthesis, device architecture, performance mechanism, energy-conversion metric, stability behaviour, toxicity issue, scalability pathway, or translational limitation; or provided foundational theoretical or review evidence necessary for interpreting photon, carrier, phonon, and interfacial energy-flow mechanisms. Priority was given to studies on photovoltaic nanomaterials, quantum dots, perovskite nanocrystals, plasmonic nanoparticles, thermoelectric superlattices, hierarchical nanocomposites, nanostructured oxides and chalcogenides,

TABLE 1 Database search strategy and scope.

Database	Representative search focus	Purpose in review
Scopus	Nano energy, photovoltaics, thermoelectrics, PV–TEG	Broad interdisciplinary coverage
Web of science	Nanostructured solar conversion, thermoelectric materials	High-impact indexed literature
ScienceDirect	Nanomaterials, device architecture, energy conversion	Materials and engineering studies
IEEE Xplore	PV–TEG systems, thermoelectric devices, energy harvesting	Device and systems engineering
ACS publications	Quantum dots, perovskites, plasmonics, interfaces	Chemistry and nanomaterial mechanisms
RSC publishing	Nanocomposites, 2D materials, stability	Materials chemistry evidence
SpringerLink	Thermoelectrics, waste heat recovery, nanostructuring	Engineering and applied energy studies
PubMed	Toxicity, nanomaterial safety, environmental health	Toxicity and safety relevance
Google scholar	Landmark and highly cited studies	Supplementary citation tracking

two-dimensional materials, carbon nanomaterials, and hybrid photovoltaic–thermoelectric platforms.

2.3.2 Exclusion criteria

Studies were excluded if they were non-peer-reviewed commentaries, editorials, patents, incomplete conference abstracts, or reports without sufficient methodological or performance information. Studies focused exclusively on bulk materials without nanoscale design relevance were excluded. Articles were also excluded if they lacked direct relevance to solar conversion, thermoelectric generation, waste-heat recovery, PV–TEG integration, or translational barriers in nano-energy systems. Outdated reports and studies lacking technological context were removed during eligibility assessment.

2.4 Study selection and screening process

The study selection process followed a PRISMA-guided workflow adapted for a systematized mini-review. Study selection was performed by the author using predefined eligibility criteria. A total of 112 records were identified through database searching. Before screening, 24 records were removed, including 19 duplicate records and 5 non-peer-reviewed records. The remaining 88 records were screened by title and abstract. During this stage, 8 records were excluded because they did not sufficiently address nano-enabled solar conversion, thermoelectric generation, PV–TEG integration, or translationally relevant material/device mechanisms. A total of 80 reports were sought for retrieval, and all were successfully retrieved. These 80 full-text reports were assessed for eligibility against the predefined criteria. Six reports were excluded at full-text assessment: 4 due to outdated content and 2 due to lack of technological context. Consequently, 74 studies were included in the final synthesis. The complete identification, screening, eligibility, and inclusion process is summarized in Figure 1.

2.5 Data extraction procedure

Data extraction was performed by the author using a structured extraction matrix to ensure consistency across included studies. Extracted variables included author and year, material class, synthesis or fabrication route, device architecture, solar or thermoelectric application, reported performance metric, stability testing approach, toxicity or sustainability concern, scalability claim, and key limitation. For solar conversion studies, extracted indicators included power conversion efficiency, light absorption behaviour, spectral response, charge transport, recombination suppression, photostability, and interface-engineering effects. For thermoelectric studies, extracted indicators included Seebeck coefficient, electrical conductivity, thermal conductivity, power factor, figure of merit, operating temperature range, and module-level relevance. For hybrid PV–TEG studies, extracted information included PV-only output, TEG-only output, integrated system output, thermal coupling strategy, operating temperature, temperature gradient, load matching, net hybrid gain, and practical deployment constraints. Each included study was further coded by publication year, application domain, nanomaterial class, dominant mechanism, and main translational limitation. Application domains were classified as solar conversion, thermoelectric generation, hybrid PV–TEG integration, interface engineering, or sustainability/scalability assessment. Dominant mechanisms included photon management, charge transport, phonon scattering, interfacial heat regulation, stability improvement, toxicity/safety relevance, and system-level integration. These coded variables were used to generate descriptive graphical summaries of the reviewed evidence.

2.6 Quality appraisal and evidence weighting

A formal meta-analytical risk-of-bias tool was not applied because the evidence base included heterogeneous experimental studies, computational studies, conceptual analyses, and review articles. Instead, each study was critically appraised according to its relevance to the review objective and the robustness of its reporting. Studies were assessed based on methodological transparency, clarity of material characterization, appropriateness of performance metrics, reproducibility of synthesis or device fabrication, inclusion of stability testing, mechanistic explanation, and discussion of scalability, toxicity, or real-world applicability. Greater interpretive weight was assigned to studies that combined performance data

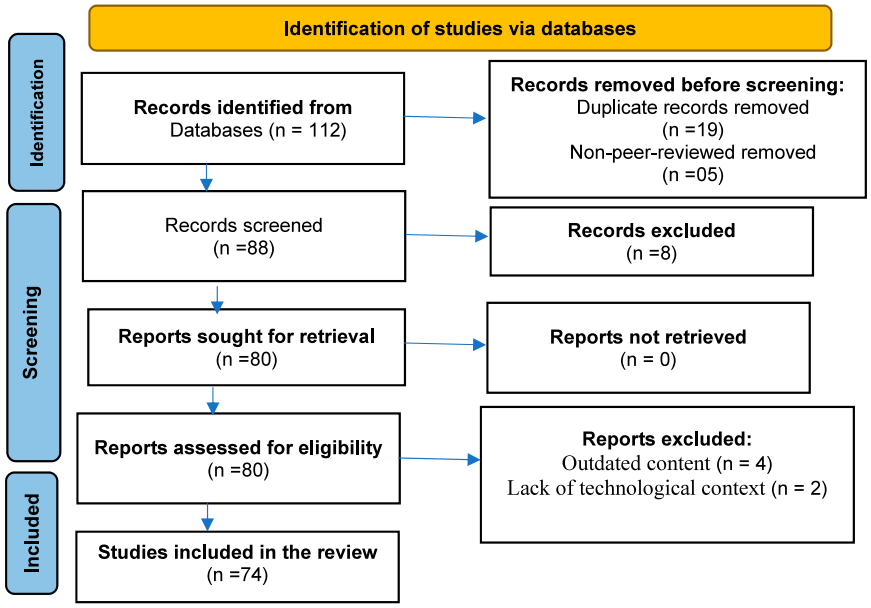


FIGURE 1
PRISMA flow diagram.

with mechanistic evidence, stability evaluation, and translational discussion. Studies reporting only peak efficiency, isolated ZT, or short-term laboratory performance without durability, toxicity, interface, or scalability assessment were interpreted cautiously.

2.7 Evidence synthesis

A narrative thematic synthesis was performed because quantitative pooling was unsuitable for the heterogeneous evidence base. The included studies differed in material composition, synthesis route, device architecture, operating conditions, performance metrics, and stability protocols. The synthesis was organized around five analytical axes: material platform, performance mechanism, device architecture, hybrid PV–TEG integration potential, and translational readiness. These axes were supported by evidence on photovoltaic losses and heat dissipation (Saeed and Zohaib, 2022; Shen et al., 2020), thermoelectric transport and ZT optimization (Shi et al., 2025; Al-Fartoos et al., 2023; Wang et al., 2026; Han et al., 2024; Bhambri and Khang, 2025; Mukherjee et al., 2022; Nandihalli, 2023), nanostructured solar absorbers and charge-transport materials (Al-Mamun, 2026; Thakur et al., 2023; Manjunatha et al., 2024; Aftab et al., 2025; Gouthaman and Thomas, 2023; Memon et al., 2026; Xue et al., 2024; Zhu et al., 2024; Gao et al., 2025; Singh J. et al., 2025; Jubair, 2026; Wang et al., 2021; Ullah et al., 2025; Zhang et al., 2025; Zhang et al., 2024), two-dimensional, carbon-based, and flexible thermoelectric materials (Fatma et al., 2024; Abu Elella et al., 2024; Mohajer et al., 2023; Pan et al., 2025; Li et al., 2026; Mannafi et al., 2026), and hybrid PV–TEG integration, photothermal coupling, and system-level benchmarking (Kim et al., 2019; Kim et al., 2020; Parkavi et al., 2026; Parkavi et al., 2025; Prabhu et al., 2026; Ibrahim et al., 2025; Xian-Long et al., 2025; Liu et al., 2026; Faddouli et al., 2024; Lehmann and Huang, 2026; Wang et al., 2025; Yousif and Jalil, 2024). In addition, descriptive graphical analysis was used to summarize the distribution of studies by application domain and major translational barrier. This analysis was not intended to estimate pooled effect sizes, but to show where the evidence is concentrated and where deployment-related gaps remain. Representative studies are summarized in Table 2 according to their focus, contribution to this review, and key translational limitations.

Descriptive analysis of the reviewed studies showed that the evidence base is concentrated mainly on solar nanomaterials, thermoelectric nanostructuring, and hybrid PV–TEG integration, with fewer studies providing full module-level validation under matched operating conditions. The main recurring translational barriers were instability, toxicity or critical-material dependence, limited scalability, contact resistance, interfacial degradation, weak module-level validation, and uncertain net hybrid gain. These distributions are summarized graphically in Figures 2, 3.

Table 1 is supported by the database coverage and disciplinary scope required for nano-enabled solar conversion, thermoelectric materials, hybrid PV–TEG systems, interface engineering, and nanomaterial safety (Shen et al., 2025; Okesiji, 2025; Eze et al., 2024; Bhagat et al., 2025; Anwar et al., 2026; Saeed and Zohaib, 2022; Shen et al., 2020; Shi et al., 2025; Eze, 2025a; Mbakaan et al., 2025; Eze et al., 2025a; Nag and Chaudhuri, 2026; Bansal et al., 2026; Singh A. K. et al., 2025; Baby et al., 2026; Boretti, 2025; Al-Fartoos et al., 2023; Manna and Ray, 2024; Xi, 2025; Aubert et al., 2022; Wang et al., 2026; Ibrahim et al., 2025; Xian-Long et al., 2025; Liu et al., 2026; Eze, 2025b; Eze et al., 2025b; Al-Mamun, 2026; Thakur et al., 2023; Manjunatha et al., 2024; Aftab et al., 2025; Gouthaman and Thomas, 2023; Memon et al., 2026; Xue et al., 2024; Zhu et al., 2024; Gao et al., 2025; Singh J. et al., 2025; Jubair, 2026; Wang et al., 2021; Ullah et al., 2025; Zhang et al., 2025; Zhang et al., 2024;

TABLE 2 Representative evidence base used for the critical synthesis of nano-enabled solar, thermoelectric, and hybrid PV–TEG systems.

Study	Main focus	Contribution to this review	Critical limitation or translational relevance
Shen et al. (2025)	Global energy transition and low-carbon pathways	Provides the broad energy-transition context for advanced renewable technologies	Policy and transition focus, not specific to nano-enabled PV–TEG integration
Okesiji (2025)	Decentralized renewable energy systems	Supports the relevance of scalable and distributed energy technologies	Limited material-level and interface-level analysis
Eze et al. (2024)	Sustainable energy policy and carbon management	Frames energy technologies within deployment and sustainability constraints	Policy-oriented rather than nanomaterial-specific
Bhagat et al. (2025)	PV systems enhanced by phase-change materials and TEGs	Supports the relevance of hybrid solar-thermal-electric systems	Highlights integration challenges but gives limited nanoscale interface analysis
Anwar et al. (2026)	Emerging photovoltaic and thermoelectric energy-harvesting trends	Provides recent context for PV and thermoelectric innovation	Broad review with limited critical comparison of toxicity and scalability
Saeed and Zohaib (2022)	Photovoltaic power losses	Supports discussion of thermalization, reflection, recombination, and resistive losses	Does not address nano-interface design directly
Shen et al. (2020)	Energy distribution and power losses in PV modules	Supports the need for heat-management and waste-heat-recovery strategies	Module-level focus rather than nanomaterial-level mechanisms
Shi et al. (2025)	Thermoelectric materials and devices	Provides basis for thermoelectric transport trade-offs, ZT, and device challenges	Shows that high ZT alone is insufficient for deployable devices
Mbakaan et al. (2025)	Nanostructured solar cells	Supports the role of nanostructuring in solar-cell efficiency improvement	Requires stronger linkage to durability, toxicity, and scalability
Nag and Chaudhuri (2026)	Nanomaterials for energy and sensing applications	Supports broad relevance of nanomaterials in energy conversion	Broad scope limits specific PV–TEG benchmarking
Bansal et al. (2026)	Quantum materials for energy harvesting	Supports the role of quantum materials in energy conversion	Emphasizes opportunity more than deployment barriers
Singh et al. (2025a)	Low-dimensional smart materials	Supports the relevance of low-dimensional materials in energy applications	Limited system-level PV–TEG analysis
Baby et al. (2026)	Nanomaterials and composites for renewable energy	Supports the role of nanocomposites in energy generation and harvesting	Broad review requiring critical filtering for this manuscript
Boretti (2025)	Zero-dimensional nanomaterials	Supports discussion of quantum dots and related 0D materials	Translation depends on toxicity, ligand stability, and device lifetime
Bjørk (2015)	Contact resistance in thermoelectric generators	Provides quantitative basis for contact-resistance limitations in TEGs	Demonstrates that contact losses can strongly reduce practical efficiency
Park et al. (2015)	Graphene-based thermal interface materials	Supports the importance of thermal interface materials	Benefits depend on contact quality, bond-line thickness, and compatibility
Huxtable et al. (2003)	Interfacial heat flow in nanotube suspensions	Supports the importance of nanoscale interfacial heat transfer	Highlights complexity of translating nanoscale thermal effects
Al-Fartoos et al. (2023)	One-dimensional thermoelectric nanostructuring	Supports nanostructuring strategies for thermoelectric performance	Scalability and module integration remain challenging
Manna and Ray (2024)	Coupled colloidal quantum-dot solids	Supports discussion of charge transport in quantum-dot systems	Ligand barriers and long-term stability remain key limitations
Xi (2025)	Carrier transfer from quantum dots to metal oxides	Supports interface-mediated charge-transfer discussion	Mechanistic insights require validation in stable devices

(*Continued*)

TABLE 2 Continued

Study	Main focus	Contribution to this review	Critical limitation or translational relevance
Aubert et al. (2022)	Size-dependent optical properties of quantum dots	Supports the quantum-confinement and spectral-tunability discussion	Optical tunability alone does not ensure safe or stable deployment
Wang et al. (2026)	Phonon engineering for thermoelectrics	Supports phonon-scattering and lattice thermal conductivity reduction	ZT improves only if carrier transport is not severely degraded
Ibrahim et al. (2025)	MPPT strategies for hybrid PV–TEG systems	Supports hybrid-system control and load-matching discussion	Net gain depends on electrical and thermal matching
Xian-Long et al. (2025)	PV–TEG hybrid receiver	Supports dual thermal management and energy-recovery concepts	Integration benefits depend on controlled heat routing
Liu et al. (2026)	Hybrid thin-film photovoltaic-absorption heat transformer system	Supports enhanced solar-energy utilization through hybridization	Requires balance between PV performance and heat utilization
Al-Mamun (2026)	Nanomaterials for solar conversion efficiency	Supports the solar-nanomaterial evidence base	Needs critical evaluation of long-term stability and scalability
Thakur et al. (2023)	Nanostructured metal chalcogenides	Supports discussion of chalcogenides, including Cd-containing systems	Cd-based chalcogenides require toxicity and environmental qualification
Manjunatha et al. (2024)	Hierarchical inorganic nanostructures for solar harvesting	Supports hierarchical morphology and solar-harvesting discussion	Large-area reproducibility remains a deployment barrier
Aftab et al. (2025)	Nanomaterials for solar-energy harvesting	Supports solar nanomaterial opportunities and challenges	Broad review requiring mechanism-specific interpretation
Gouthaman and Thomas (2023)	Metal oxide nanostructures as electron-transport layers	Supports the role of metal oxides in charge extraction	Performance depends on defects, passivation, and interfacial alignment
Memon et al. (2026)	Photoanode design for dye-sensitized solar cells	Supports nanostructured photoanode discussion	Translation depends on stability and scalable fabrication
Xue et al. (2024)	Charge trapping in semiconductor photocatalysts	Supports discussion of trap states and recombination	Shows that high surface area may increase recombination pathways
Zhu et al. (2024)	Quantum-dot tandem solar cells	Supports use of quantum dots in tandem architectures	Toxicity and ligand-limited charge transport remain barriers
Gao et al. (2025)	Narrow-bandgap infrared quantum-dot solar cells	Supports quantum-dot spectral extension	Heavy-metal composition and long-term stability limit translation
Singh et al. (2025b)	Quantum-dot-sensitized solar cells	Supports quantum-dot sensitization strategies	Requires stronger operational lifetime evidence
Wang et al. (2021)	Ligand-capped colloidal nanocrystals	Supports ligand chemistry and charge-transport discussion	Ligand exchange and film reproducibility remain central barriers
Ullah et al. (2025)	Perovskite nanocrystals, quantum dots, and 2D structures	Supports perovskite nanocrystal and quantum-confined material discussion	Heat, moisture, ion migration, and Pb toxicity remain major concerns
Zhang et al. (2025)	Surface chemistry-engineered perovskite quantum-dot photovoltaics	Supports surface passivation and interface engineering	Long-term stability and scalable encapsulation remain unresolved
Zhang et al. (2024)	Halide perovskite nanostructure engineering	Supports perovskite nanostructuring and photocatalytic/solar relevance	Practical use requires heat, moisture, and ion-migration control
Faddouli et al. (2024)	Solar, thermal, photovoltaic, and thermoelectric hybrid systems	Supports hybrid PV–TEG and solar-thermal integration discussion	System-level benefit requires net-gain validation, packaging, and heat-sink assessment

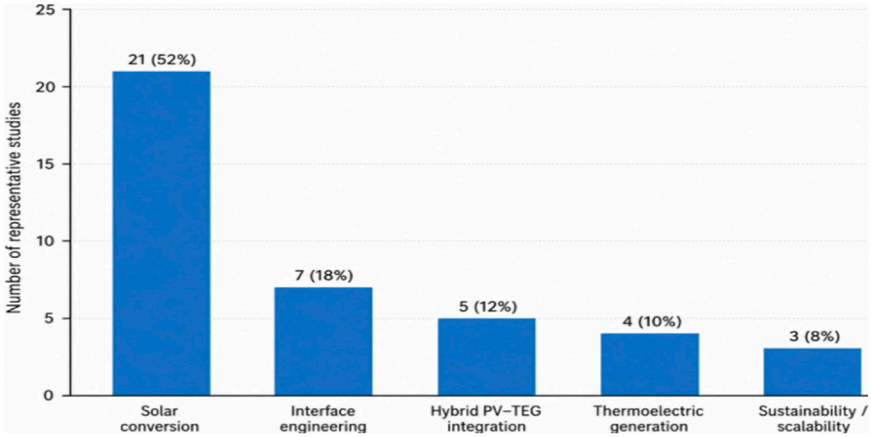


FIGURE 2
Distribution of included studies by dominant application domain representative evidence of n= 40.

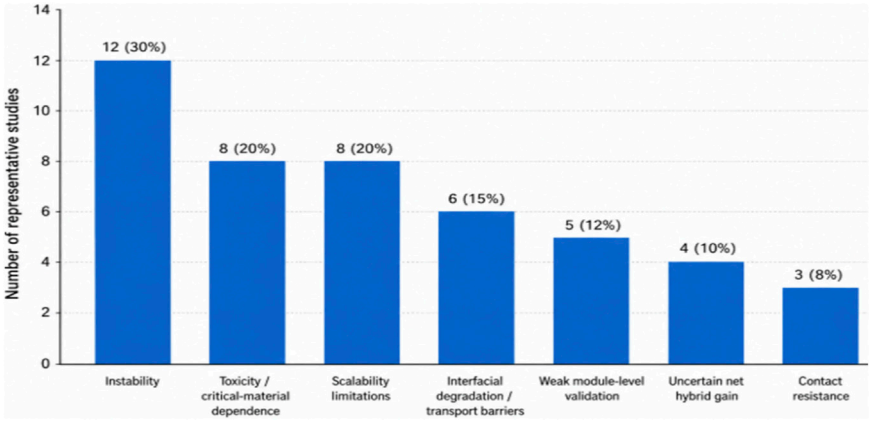


FIGURE 3
Distribution of major translational barriers identified across the included studies based on representative evidence of n = 40.

Fatma et al., 2024; Abu Elella et al., 2024; Mohajer et al., 2023; Han et al., 2024; Bhambri and Khang, 2025; Mukherjee et al., 2022; Nandihalli, 2023; Pan et al., 2025; Li et al., 2026; Mannafi et al., 2026; Faddouli et al., 2024; Chen et al., 2026; Zhao et al., 2025; An et al., 2023; Lehmann and Huang, 2026). Table 2 summarizes representative studies selected from the final evidence pool to support the critical synthesis across energy-transition context (Shen et al., 2025; Okesiji, 2025; Eze et al., 2024; Bhagat et al., 2025; Anwar et al., 2026), photovoltaic losses (Saeed and Zohaib, 2022; Shen et al., 2020), thermoelectric transport (Shi et al., 2025; Al-Fartoos et al., 2023; Wang et al., 2026; Han et al., 2024; Bhambri and Khang, 2025; Mukherjee et al., 2022; Nandihalli, 2023), solar nanomaterials (Al-Mamun, 2026; Thakur et al., 2023; Manjunatha et al., 2024; Aftab et al., 2025; Gouthaman and Thomas, 2023; Memon et al., 2026; Xue et al., 2024; Zhu et al., 2024; Gao et al., 2025; Singh J. et al., 2025; Jubair, 2026; Wang et al., 2021; Ullah et al., 2025; Zhang et al., 2025; Zhang et al., 2024), two-dimensional/flexible thermoelectrics (Fatma et al., 2024; Abu Elella et al., 2024; Mohajer et al., 2023; Pan et al., 2025; Li et al., 2026; Mannafi et al., 2026), and hybrid PV–TEG integration (Ibrahim et al., 2025; Xian-Long et al., 2025; Liu et al., 2026; Eze, 2025b; Eze et al., 2025b; Al-Mamun, 2026; Thakur et al., 2023; Manjunatha et al., 2024; Aftab et al., 2025; Gouthaman and Thomas, 2023; Memon et al., 2026; Xue et al., 2024; Zhu et al., 2024; Faddouli et al., 2024; Lehmann and Huang, 2026; Wang et al., 2025; Yousif and Jalil, 2024).

2.8 Reliability, transparency, and methodological limitations

The representative studies summarized in Table 2 were used to strengthen the transparency of the narrative synthesis and to show how the critical interpretation was grounded in the reviewed evidence base. Reliability was strengthened through the use of multiple databases, explicit eligibility criteria, structured data extraction, PRISMA-guided screening, and transparent reporting of inclusion and exclusion decisions. These steps reduced selection bias and improved reproducibility while remaining appropriate

for a critical mini-review. However, several limitations should be acknowledged. First, screening and data extraction were performed by a single author, which may introduce selection or interpretation bias despite the use of predefined criteria and a structured extraction matrix. Second, the review was limited to English-language publications, which may exclude relevant studies published in other languages. Third, database coverage may have introduced indexing bias, particularly for emerging preprint or regional literature. Fourth, the synthesis was qualitative because the field contains substantial heterogeneity in nanomaterial platforms, device architectures, test conditions, and performance metrics. Fifth, because the review emphasized mechanistic and translational relevance, some technically relevant studies may have been excluded if they lacked sufficient connection to solar conversion, thermoelectric generation, hybrid PV–TEG integration, or nano-energy deployment.

3 Thematic synthesis and critical discussion

3.1 Scientific basis of interface-programmed nano energy systems

Nano-energy systems exhibit size-dependent behaviour when material dimensions become comparable to characteristic physical length scales; however, each length scale is associated with a different physical mechanism. Dimensions approaching the exciton Bohr radius mainly produce quantum confinement effects, which modify electronic band structure and optical transition energies. Dimensions comparable to the carrier diffusion length affect charge transport by influencing carrier separation, collection, and recombination. When dimensions approach the phonon mean free path, thermal transport is altered through enhanced boundary scattering and phonon confinement. Similarly, dimensions comparable to the optical skin depth affect light absorption by controlling electromagnetic field penetration and optical energy localization (Al-Fartoos et al., 2023; Manna and Ray, 2024). In this size regime, energy conversion is controlled not only by bulk composition, but also by quantum confinement, surface chemistry, grain boundaries, defect states, heterojunctions, and interfacial thermal resistance (Xi, 2025). These nanoscale effects are directly relevant to photovoltaic–thermoelectric integration because solar photons, photogenerated carriers, rejected heat, and phonons must be managed within a single energy-flow pathway (Al-Fartoos et al., 2023; Xi, 2025). In the photovoltaic component, nanostructuring improves solar conversion by tuning band gaps, enhancing light absorption, suppressing recombination, and improving charge extraction. Quantum dots provide size-dependent absorption and spectral tunability; perovskite nanocrystals offer strong absorption and defect-tolerant charge transport; plasmonic nanoparticles enhance local electromagnetic fields and light trapping; while two-dimensional materials and carbon nanostructures can function as transport layers, electrodes, or interfacial modifiers (Aubert et al., 2022). However, these advantages are counterbalanced by nanoscale vulnerabilities, including trap-state formation, ion migration, oxidation, ligand-induced transport barriers, lead or cadmium toxicity, and instability under heat, moisture, oxygen, and illumination.

In the thermoelectric component, nanostructuring is used to improve the balance between the Seebeck coefficient, electrical conductivity, and thermal conductivity (Al-Fartoos et al., 2023). Superlattices, nanoinclusions, hierarchical nanocomposites, and two-dimensional thermoelectric materials reduce lattice thermal conductivity by scattering phonons at multiple length scales, while energy filtering at interfaces can improve carrier selectivity (Shi et al., 2025; Wang et al., 2026). These mechanisms are central to increasing thermoelectric figure of merit and enabling waste-heat recovery from photovoltaic modules. However, thermoelectric nanostructures also face practical barriers, including contact resistance, brittle interfaces, thermal cycling degradation, rare-element dependence, and difficulty scaling complex architectures into stable modules (Al-Fartoos et al., 2023; Wang et al., 2026). For hybrid PV–TEG systems, the critical scientific issue is not simply combining a photovoltaic layer with a thermoelectric module. The main challenge is controlling the interface between solar electricity generation and heat recovery (Al-Fartoos et al., 2023; Xian-Long et al., 2025). A photovoltaic absorber converts part of the solar spectrum into electrical current but dissipates substantial energy as heat through thermalization, non-radiative recombination, and resistive losses (Liu et al., 2026; Eze, 2025b). If this heat is poorly managed, it raises cell temperature and reduces photovoltaic efficiency. If it is effectively routed through a thermoelectric stage while preserving a sufficient temperature gradient, it can contribute to additional electrical output (Ibrahim et al., 2025; Eze, 2025b).

Therefore, interface programming becomes the central design principle. Optical interfaces must enhance photon capture without excessive parasitic absorption. Electronic interfaces must extract carriers while minimizing recombination. Thermal interfaces must direct heat toward the thermoelectric leg while maintaining a usable temperature difference. Mechanical and chemical interfaces must remain stable under thermal cycling, illumination, humidity, and long-term operation. This coupled control of photons, carriers, phonons, and interfaces distinguishes interface-programmed nano energy systems from conventional nanomaterial-based solar or thermoelectric devices.

Accordingly, the scientific foundation of this review is that high-performance nano energy systems cannot be evaluated by efficiency or ZT alone. For rigorous evaluation, material performance must be interpreted together with interfacial energy-flow control, operational stability, toxicity risk, and scalable device integration. This framework provides the basis for comparing quantum dots, perovskite nanostructures, plasmonic nanoparticles, superlattices, hierarchical nanocomposites, and two-dimensional materials in later sections.

3.2 Nanomaterials for solar energy conversion

Nanomaterials for solar energy conversion are valuable because they allow photon absorption, charge separation, carrier transport, and interfacial recombination to be controlled at length scales relevant to photovoltaic operation (Al-Mamun, 2026). In the context of interface-programmed nano energy systems, their importance is not limited to improving power conversion efficiency. Their

wider role is to regulate how incident photons are absorbed, how photogenerated carriers are extracted, and how residual heat is transferred toward possible thermoelectric recovery.

3.2.1 Semiconductor nanostructures

Semiconductor nanostructures such as titanium dioxide, zinc oxide, tin oxide, cadmium sulfide, and related metal oxides or chalcogenides remain important platforms for solar conversion because they provide tunable morphology, high surface area, controllable optical response, and charge-transfer pathways (Thakur et al., 2023; Manjunatha et al., 2024). However, Cd-based chalcogenides such as CdS require careful qualification. Although CdS can provide favorable band alignment, visible-light absorption, and charge-transfer properties in sensitized, heterojunction, and photoelectrochemical solar architectures, its cadmium content creates important toxicity, environmental, regulatory, and end-of-life concerns. Therefore, Cd-containing semiconductor nanostructures should be evaluated not only by their optical or electronic performance, but also by encapsulation reliability, leakage risk, recyclability, safer processing routes, and the feasibility of lower-toxicity alternatives. Nanotubes, nanowires, nanosheets, mesoporous films, and hierarchical porous structures can shorten carrier transport distances, increase absorber contact area, and improve electron or hole extraction at device interfaces (Aftab et al., 2025).

In dye-sensitized, quantum-dot-sensitized, perovskite, photoelectrochemical, and hybrid solar cells, these nanostructures often function as electron transport layers, scaffold materials, photoanodes, interfacial modifiers, or catalytic surfaces (Gouthaman and Thomas, 2023; Memon et al., 2026). Their nanoscale geometry can enhance light harvesting and carrier collection, but the same high surface area can also increase defect density, surface traps, and recombination pathways. Therefore, their performance depends strongly on surface passivation, defect control, crystallinity, dopant regulation, and interfacial energy alignment (Xue et al., 2024).

For hybrid PV–TEG systems, semiconductor nanostructures are especially relevant when they improve solar absorption while limiting parasitic heating and interfacial charge loss. Future studies should therefore report not only efficiency improvement, but also recombination resistance, thermal stability, interfacial degradation, toxicity or leakage risk for Cd-containing chalcogenides, and compatibility with downstream heat-management layers.

3.2.2 Quantum dots

Quantum dots offer size-tunable bandgaps, strong absorption coefficients, solution processability, and potential multiple exciton generation, making them attractive for tandem solar cells, sensitized solar cells, luminescent solar concentrators, and spectral-management layers (Zhu et al., 2024; Gao et al., 2025). Their main advantage is that optical response can be tuned by controlling particle size, composition, surface chemistry, and ligand environment (Gao et al., 2025; Singh J. et al., 2025). This makes them particularly useful for harvesting specific regions of the solar spectrum and for designing wavelength-selective interfaces in hybrid solar architectures.

In interface-programmed nano energy systems, quantum dots can contribute to photon management by broadening absorption, enhancing spectral matching, and enabling semi-transparent or tandem configurations (Jubair, 2026). However, their translation is constrained by cadmium and lead toxicity, ligand-induced barriers to charge transport, oxidation, photobleaching, aggregation, and limited long-term operational stability. Colloidal ligands that stabilize particles during synthesis may also impede carrier mobility in solid-state devices unless carefully exchanged or engineered (Wang et al., 2021).

For translational relevance, future quantum-dot solar studies should move beyond reporting tunable absorption or short-term efficiency. They should demonstrate heavy-metal-free or reduced-toxicity compositions, stable ligand chemistry, reproducible film formation, realistic illumination testing, and device-level lifetime data under heat, oxygen, moisture, and continuous operation.

3.2.3 Perovskite nanocrystals and quantum-confined perovskites

Perovskite nanocrystals and quantum-confined perovskites are among the most dynamic materials for solar conversion because they combine strong optical absorption, defect-tolerant electronic structure, tunable composition, long carrier diffusion potential, and low-temperature processability (Ullah et al., 2025). Nanoscale control can improve grain growth, suppress non-radiative recombination, passivate surface defects, regulate ion migration, and tune interfacial energy alignment with transport layers (Zhang et al., 2025). Their importance for interface-programmed solar systems lies in their dual sensitivity and tunability. Properly engineered perovskite nanostructures can improve light harvesting and carrier extraction, while poorly controlled surfaces and grain boundaries can accelerate degradation (Zhang et al., 2024). Moisture, oxygen, heat, illumination, electrical bias, and ion migration remain major threats to long-term device operation. Lead toxicity also remains a major translational barrier, especially for large-area deployment and end-of-life management.

For hybrid PV–TEG systems, perovskite nanostructures are attractive because of their low-temperature fabrication, strong optical absorption, tunable bandgap, and potential compatibility with tandem or flexible architectures. However, their practical compatibility with PV–TEG integration should not be overstated because a thermal mismatch can arise between the photovoltaic and thermoelectric components. Perovskite absorbers are sensitive to heat, moisture, oxygen, illumination, and electrical bias, whereas the thermoelectric stage requires a useful temperature gradient to generate meaningful output. If residual heat is allowed to accumulate at the perovskite absorber or poorly controlled PV–TEG interface, it can accelerate ion migration, defect formation, interfacial degradation, and loss of photovoltaic performance. Therefore, perovskite-based PV–TEG architectures require thermal-management strategies that recover heat without thermally overstressing the perovskite layer. Spectral splitting can direct high-energy photons to photovoltaic conversion while routing sub-bandgap or infrared radiation toward thermal or thermoelectric recovery. Thermal decoupling or selective heat-routing layers can help maintain a temperature gradient across the TEG while limiting heat backflow into the perovskite absorber. Strong encapsulation,

thermally stable transport layers, ion-migration suppression, and moisture/oxygen barriers are also essential for maintaining stability under coupled heat, light, humidity, and bias stress. Thus, future work should demonstrate not only perovskite PV efficiency, but also photovoltaic operating temperature, TEG temperature difference, encapsulation durability, interfacial thermal stability, and net hybrid power gain under realistic PV–TEG operating conditions.

3.2.4 Plasmonic nanoparticles

Plasmonic nanoparticles, including gold, silver, aluminum, and copper-based nanostructures, improve solar conversion by concentrating electromagnetic fields, increasing scattering, extending optical path length, and enhancing absorption in thin active layers (Indhu et al., 2024; Joshi et al., 2022). Their value is strongest in devices where absorber thickness must be minimized for flexibility, cost reduction, transparency, or improved carrier extraction. Within an interface-programmed framework, plasmonic structures can act as photon-management layers that redirect or intensify incident light before it reaches the active absorber. They may also support spectral selectivity in hybrid PV–TEG systems by enhancing useful absorption while potentially influencing local heat generation. However, this benefit is highly design-dependent. Poorly positioned plasmonic particles can introduce parasitic absorption, local overheating, chemical instability, recombination sites, or optical losses.

Gold and silver offer strong plasmonic response but are expensive and may be chemically unstable in some device environments (Hang et al., 2024; Gao et al., 2026). Aluminum and copper are more abundant but require careful oxidation control (Tannyan et al., 2002). Therefore, plasmonic solar studies should clearly distinguish between genuine photocurrent enhancement and heat-induced or optical artefacts. For translational relevance, future work should report nanoparticle stability, cost implications, large-area reproducibility, and whether plasmonic heating improves or harms net device output.

3.2.5 Carbon, polymeric, and two-dimensional nanomaterials

Carbon-based, polymeric, and two-dimensional nanomaterials, including graphene, carbon nanotubes, MXenes, transition-metal dichalcogenides, graphitic carbon nitride, conductive polymers, and hybrid nanocomposites, are increasingly important as transport layers, electrodes, interfacial modifiers, flexible substrates, and stability-enhancing additives in solar energy devices (Fatma et al., 2024; Abu Elella et al., 2024). Their value lies less in functioning as universal standalone absorbers and more in their ability to regulate interfaces.

Graphene and carbon nanotubes can improve conductivity, mechanical flexibility, and charge extraction. MXenes provide tunable surface chemistry and high conductivity but may suffer from oxidation and restacking (Mohajer et al., 2023). Transition-metal dichalcogenides offer thickness-dependent electronic properties and potential catalytic or transport functionality. Conductive polymers can improve flexibility and processability, although their stability and conductivity may be lower than inorganic alternatives. Graphitic carbon nitride and hybrid carbon systems can contribute to photocatalytic and interfacial charge-transfer applications.

In hybrid PV–TEG architectures, these materials are particularly relevant because they can bridge optical, electrical, thermal, and mechanical functions. They may serve as flexible electrodes, thermal interface modifiers, charge-selective layers, protective coatings, or mechanically compliant interconnects. Their translational barriers include batch-to-batch variability, oxidation, dispersion difficulty, interfacial incompatibility, and inconsistent large-area film quality.

Therefore, their greatest opportunity is not as "miracle materials," but as programmable interfaces that improve carrier extraction, suppress recombination, enhance environmental stability, and support mechanical integration. To unify these material classes within the mechanism-to-translation perspective of this review, their dominant pathways and barriers are summarized in Figure 4.

3.3 Nanoengineered thermoelectric systems

Thermoelectric performance is governed by the dimensionless figure of merit as shown in Equation 1

$$ZT = \frac{S^2 \sigma T}{\kappa} \tag{1}$$

where (S) is the Seebeck coefficient, (σ) is the electrical conductivity, (T) is the absolute temperature, and (κ) is the total thermal conductivity. The central materials challenge is that these transport parameters are strongly interdependent. Increasing carrier concentration may improve electrical conductivity but can reduce the Seebeck coefficient, while strategies that suppress thermal conductivity may also disrupt carrier mobility. This coupling makes thermoelectric optimization a problem of selective transport control rather than simple materials enhancement (Han et al., 2024).

Nanostructuring provides one of the most effective routes for controlling this trade-off. Interfaces, grain boundaries, nanoprecipitates, defects, and low-dimensional structures can scatter heat-carrying phonons more strongly than charge carriers, thereby reducing lattice thermal conductivity while preserving useful electronic transport (Bhambri and Khang, 2025). For photovoltaic-thermoelectric integration, this distinction is critical: the thermoelectric stage must convert residual photovoltaic heat into electricity without introducing excessive thermal resistance, contact losses, or instability under repeated solar heating and cooling cycles.

3.3.1 Superlattices and low-dimensional thermoelectrics

Superlattices and quantum-well structures are foundational examples of thermoelectric interface engineering. Their periodic interfaces scatter phonons and modify the electronic density of states, creating opportunities to reduce thermal conductivity while enhancing carrier selectivity (Mukherjee et al., 2022). In this sense, they provide a mechanistic model for the interface-programmed strategy proposed in this review. However, their practical value for hybrid photovoltaic-thermoelectric systems is constrained by complex fabrication, high processing cost, limited

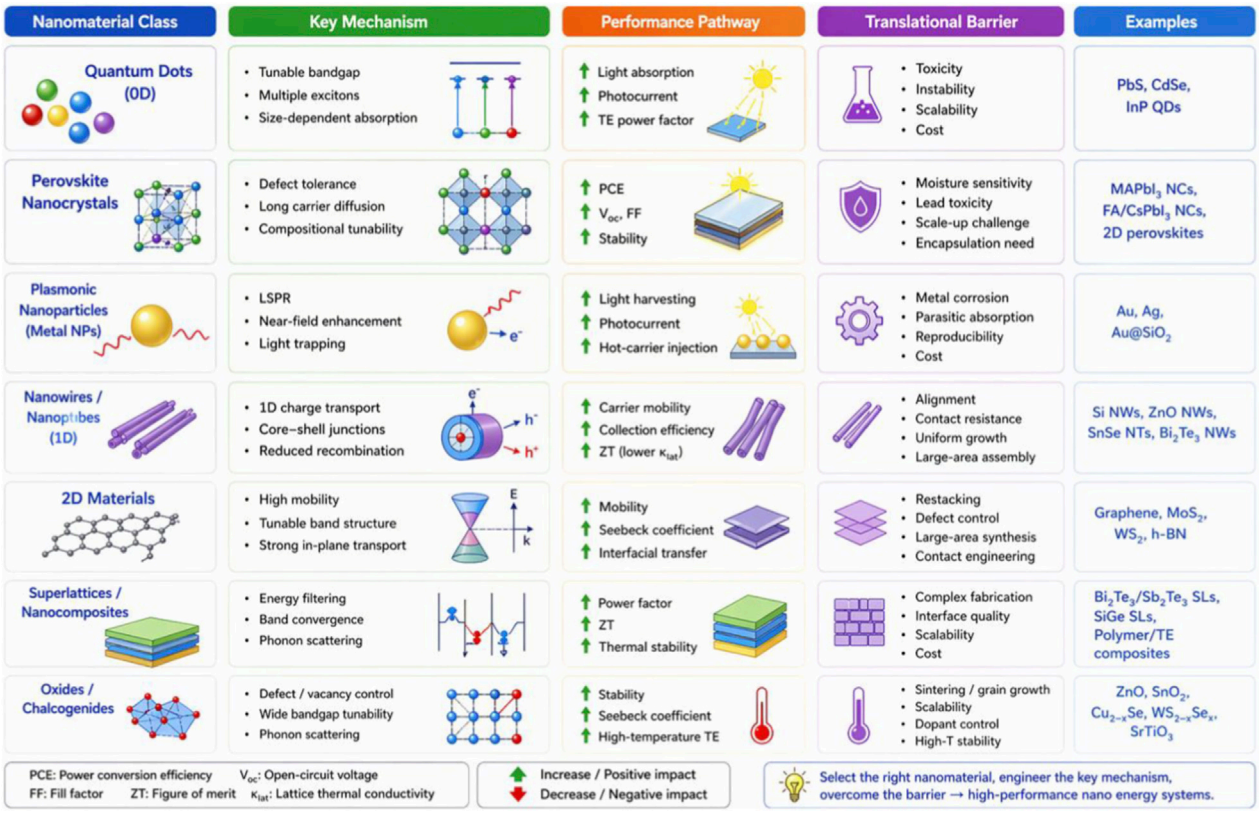


FIGURE 4
Mechanism map linking nanomaterial classes to dominant performance pathways and key translational barriers in nano energy systems.

active volume, and instability at repeated thermal interfaces. Although superlattices may not always be the most scalable thermoelectric platform, they remain important because they demonstrate how engineered interfaces can separate heat flow from charge transport.

3.3.2 Nanocomposites and hierarchical architectures

Nanocomposites and hierarchical thermoelectric architectures improve thermoelectric performance by introducing phonon-scattering centres across a broad structural hierarchy rather than relying on a single defect type (Al-Fartoos et al., 2023; Nandihalli, 2023). At the atomic scale, point defects such as vacancies, dopants, alloying disorder, antisite defects, and mass-fluctuation sites, typically below approximately 1 nm, scatter short-wavelength phonons. At the nanoscale, nanoprecipitates, nanoinclusions, embedded second phases, coherent or semi-coherent interfaces, and endotaxial nanostructures, commonly within the ~1–100 nm range, scatter mid-wavelength phonons while also creating potential energy-filtering barriers for charge carriers when band alignment is favourable. At the mesoscale, grain boundaries, dislocations, pores, lamellae, and hierarchical grains, often from ~100 nm to several micrometres, scatter longer-wavelength phonons and further reduce lattice thermal conductivity. This multiscale defect architecture is particularly relevant to bismuth telluride, lead telluride, tin selenide, skutterudites, half-Heusler alloys, copper chalcogenides, and polymer-based thermoelectrics because these systems require broad-spectrum phonon suppression without destroying electronic percolation pathways. In an optimized hierarchy, lattice thermal conductivity is reduced through cumulative phonon scattering, while electrical conductivity and carrier mobility are preserved through connected conducting phases, controlled grain-boundary chemistry, and limited carrier-blocking barriers. The resulting improvement in thermoelectric figure of merit, ZT, therefore depends not simply on increasing defect density, but on selectively scattering phonons more strongly than charge carriers. For photovoltaic–thermoelectric integration, this distinction is critical because the thermoelectric stage must sustain a usable temperature gradient and convert low-grade photovoltaic heat without introducing excessive contact resistance, brittle interfaces, or thermal-cycling instability. However, hierarchical complexity also introduces translational barriers, including phase segregation, interfacial degradation, grain-growth instability, reproducibility problems, contact resistance, and thermal fatigue. Therefore, nanocomposite thermoelectrics should be assessed not only by peak ZT, but also by the reported phonon-scattering hierarchy, lattice thermal conductivity reduction, carrier mobility retention, module-level power density, temperature-gradient stability, contact durability, and compatibility with photovoltaic operating conditions.

3.3.3 Two-dimensional and flexible thermoelectrics

Two-dimensional materials and carbon-based thermoelectrics are attractive for lightweight, flexible, and conformable energy systems (Li et al., 2026). Graphene, carbon nanotubes, MXenes, transition-metal dichalcogenides, and conductive polymers can support flexible thermoelectric devices for low-grade heat harvesting, wearable electronics, self-powered sensors, and mechanically compliant hybrid energy systems (Li et al., 2026). Although their thermoelectric performance is often lower than that of optimized inorganic bulk materials, their advantage lies in integration. They can conform to curved surfaces, tolerate mechanical deformation, and serve as interfacial layers between photovoltaic modules and thermoelectric components (Mannafi et al., 2026). This makes them relevant to interface-programmed nano energy systems, where mechanical contact, thermal coupling, and interfacial stability are as important as the intrinsic Seebeck coefficient or electrical conductivity. Future studies on flexible thermoelectrics should therefore report device-level output under realistic temperature gradients, mechanical cycling, thermal cycling, humidity, oxidation resistance, and integration behaviour with photovoltaic or photothermal components. The material-level Seebeck coefficient alone is insufficient to establish practical relevance for hybrid energy harvesting. Representative nano energy materials, their dominant performance pathways, advantages, and translational limitations are summarized in Table 3.

To operationalize the stability–toxicity–scalability trilemma as a critical evaluation tool, the material platforms summarized in Table 3 were further assessed using a semi-quantitative scoring matrix. Each platform was assigned a score from 1 to 5 for stability, toxicity/safety, and scalability as shown in Table 3. A score of 1 indicates a severe translational limitation, 3 indicates a moderate or strongly condition-dependent limitation, and 5 indicates a comparatively favorable attribute. For toxicity/safety, a higher score indicates lower toxicity, lower environmental concern, or fewer regulatory constraints. The scores are not intended as absolute material rankings because each class includes diverse compositions, synthesis routes, encapsulation strategies, and device architectures. Rather, they provide a content-specific screening framework based on the dominant limitations reported for each nanomaterial class in solar, thermoelectric, and hybrid PV–TEG, applications.

The scoring matrix in Table 4 shows that the stability–toxicity–scalability trilemma functions as a material-specific screening tool rather than a general conceptual statement. Quantum dots and perovskite nanocrystals are attractive for spectral tunability and high photovoltaic potential, but their lower scores are driven by degradation sensitivity, ligand or ion-migration problems, and Pb/Cd-related concerns. Plasmonic nanoparticles can improve light management, but their translational value depends on whether near-field enhancement outweighs parasitic absorption, local heating, cost, and oxidation. Superlattices provide strong mechanistic control of phonon transport, but their low scalability score reflects fabrication complexity and limited module-level practicality. Carbon nanomaterials and nanostructured oxides show stronger stability or safety profiles, but still require reproducible large-area processing and device-level validation. Hybrid PV–TEG nanostructures receive the lowest combined translational readiness because their performance depends on coupled device operation, including heat routing, PV temperature control, TEG temperature-gradient preservation, contact resistance, packaging, and verified net system-level gain.

3.4 Hybrid photovoltaic–thermoelectric nano energy platforms

Hybrid photovoltaic–thermoelectric systems are designed to improve total solar-energy utilization by converting both direct photovoltaic electricity and residual heat into useful electrical output (Faddouli et al., 2024). In these systems, the photovoltaic component converts absorbed photons into electrical carriers, while the thermoelectric component converts part of the remaining temperature gradient into additional power. The scientific value of this architecture lies in its ability to treat photovoltaic heat not only as a loss pathway, but also as a secondary energy resource. However, practical performance gains are not guaranteed by simply attaching a thermoelectric generator to the back of a photovoltaic cell. The net output depends on how effectively the system manages optical transmission, photon absorption, carrier extraction, heat localization, thermal-gradient preservation, electrical load matching, contact resistance, and device packaging. If the thermoelectric layer traps heat near the photovoltaic absorber without maintaining an adequate temperature difference across the thermoelectric legs, the photovoltaic temperature may rise, and the total device output may decrease. Therefore, hybrid PV–TEG performance must be judged by net energy gain, not by the isolated performance of either subsystem.

In this context, gross output refers to the simple addition of photovoltaic and thermoelectric power outputs, whereas net hybrid gain refers to the actual increase in usable system-level power after accounting for thermal losses, photovoltaic temperature rise, contact resistance, load mismatch, heat-sink requirements, and added system complexity. The central design challenge is therefore interface programming. Optical interfaces must direct useful photons into the photovoltaic absorber while minimizing reflection and parasitic absorption (Chen et al., 2026). Electrical interfaces must extract carriers efficiently without increasing recombination or series resistance. Thermal interfaces must route residual heat toward the thermoelectric module while preserving a temperature gradient across the thermoelectric legs. Mechanical interfaces must remain stable under repeated expansion, contraction, humidity exposure, illumination, and thermal cycling (Zhao et al., 2025). In this architecture, the interface is not a passive contact region; it is the control point that determines whether photon, carrier, and phonon pathways cooperate or compete.

Nanomaterials can contribute to hybrid PV–TEG platforms through several specific functions. Selective absorbers and spectrally engineered coatings can improve photon management and reduce optical losses. Plasmonic and photothermal nanostructures can localize or redistribute heat, although they must be designed carefully to avoid damaging photovoltaic performance. Nanofluids can improve heat extraction in photovoltaic–thermal configurations and create more favorable thermal gradients for thermoelectric conversion. Low-thermal-conductivity thermoelectric nanocomposites can suppress phonon transport while maintaining electrical conduction. Carbon materials, MXenes,

TABLE 3 Representative nano energy material platforms: primary functions and translational limitations.

Nanomaterial platform	Primary role in nano energy systems	Dominant functional mechanism	Main advantage	Key translational limitation
Quantum dots	Solar absorbers, sensitizers, tandem layers, spectral converters	Quantum confinement, bandgap tunability, broad-spectrum absorption	Tunable optical response and solution processability	Pb/Cd toxicity, ligand-limited charge transport, photochemical instability
Perovskite nanocrystals	Photovoltaic absorbers and tandem solar layers	Defect tolerance, strong absorption, tunable composition, carrier transport	High efficiency potential and low-temperature fabrication	Moisture, heat, oxygen, light instability, ion migration, Pb toxicity
Plasmonic nanoparticles	Light-management and spectral-enhancement layers	Localized surface plasmon resonance, near-field enhancement, light scattering	Improved absorption in thin active layers	Parasitic heating, noble-metal cost, oxidation, reproducibility
Nanowires and nanotubes	Charge-transport pathways, photoelectrodes, flexible interfaces	One-dimensional carrier transport, shortened diffusion pathways, boundary phonon scattering	Directional transport and improved carrier collection	Alignment, contact resistance, large-area assembly
Two-dimensional materials and MXenes	Electrodes, transport layers, interfacial modifiers, flexible components	High mobility, tunable surface chemistry, interfacial charge regulation	Conductive, flexible, multifunctional interfaces	Oxidation, restacking, flake variability, scale-up inconsistency
Superlattices	Thermoelectric thin films and model interface systems	Periodic interface phonon scattering, density-of-states modification	Strong suppression of lattice thermal conductivity	Complex fabrication, high cost, limited scalability
Hierarchical nanocomposites	Thermoelectric modules and heat-recovery materials	Multiscale phonon scattering, energy filtering, defect engineering	Improved ZT through partial decoupling of heat and charge transport	Processing complexity, phase stability, thermal-cycling degradation
Nanostructured oxides and chalcogenides	Solar absorbers, photoelectrodes, thermoelectrics	Defect engineering, oxygen-vacancy control, phonon scattering	Chemical stability and tunable optical/electronic transport	Lower conductivity, dopant control, sintering and reproducibility challenges
Carbon nanomaterials	Electrodes, transport layers, flexible energy devices, interconnects	High conductivity, mechanical flexibility, interfacial charge transfer	Lightweight and mechanically compliant integration	Dispersion difficulty, variable film quality, inconsistent performance
Hybrid PV–TEG nanostructures	Coupled solar electricity generation and waste-heat recovery	Sequential photon-to-electricity and heat-to-electricity conversion	Higher total energy-utilization potential	Thermal matching, packaging, contact resistance, cost, uncertain net gain

conductive polymers, and flexible two-dimensional materials can serve as mechanically compliant electrodes, thermal interface layers, or interconnects (An et al., 2023).

Several hybrid architectures are especially relevant to interface-programmed nano energy design. Spectral-splitting PV–TEG systems separate high-energy photons for photovoltaic conversion and direct lower-energy or thermal components toward thermoelectric recovery (Lehmann and Huang, 2026). Photovoltaic–thermal–thermoelectric systems use cooling channels or nanofluids to remove heat from the photovoltaic module while creating a controlled thermal input for the thermoelectric stage. Perovskite–silicon tandem modules coupled with thermoelectrics offer high photovoltaic absorption but require careful thermal management because perovskites are sensitive to heat, moisture, oxygen, and ion migration. Photothermal absorber–TEG systems are useful where heat generation is intentional, while self-powered sensor platforms can combine photovoltaics, thermoelectrics, and storage for autonomous low-power operation.

The main weakness in the current hybrid PV–TEG literature is that many studies report added thermoelectric output without proving true system-level improvement. A rigorous hybrid study should compare photovoltaic-only, thermoelectric-only, and integrated PV–TEG outputs under identical illumination, ambient temperature, heat-sink conditions, and electrical loading. It should also report photovoltaic temperature, thermoelectric temperature difference, contact resistance, conversion efficiency, device area, stability under cycling, and net power gain after accounting for added thermal and electrical losses.

Accordingly, the future of hybrid photovoltaic–thermoelectric nano energy platforms depends less on physical stacking and more on coordinated interface design. The most promising systems will be those that can simultaneously enhance photon absorption, preserve

TABLE 4 Semi-quantitative stability–toxicity–scalability scoring of representative nano-energy material platforms.

Nanomaterial platform	Stability score	Toxicity/Safety score	Scalability score	Basis for scoring and translational interpretation
Quantum dots	2	2	3	The low stability score reflects oxidation, aggregation, photobleaching, surface-trap formation, and ligand-dependent charge-transport barriers. The low toxicity/safety score is mainly due to Pb- and Cd-based quantum dots, although InP and other heavy-metal-reduced systems improve this profile. Scalability is moderate because colloidal synthesis and solution processing are attractive, but ligand exchange, film cracking, batch uniformity, and long-term device stability remain unresolved.
Perovskite nanocrystals	2	2	3	The stability score is limited by moisture, oxygen, heat, illumination, ion migration, and surface-defect-driven degradation. The toxicity/safety score remains low because many high-performing perovskite systems still rely on Pb-containing compositions. Scalability is moderate because low-temperature processing is promising, but large-area coating uniformity, encapsulation reliability, thermal tolerance, and end-of-life Pb management remain major barriers.
Plasmonic nanoparticles	3	3	3	Stability is moderate because plasmonic response depends on particle size, shape, spacing, oxidation state, and chemical compatibility with the absorber. Toxicity/safety is moderate because Au and Ag are relatively less toxic but costly and resource-intensive, while Cu and Al are more abundant but oxidation-prone. Scalability is moderate because reproducible large-area nanoparticle placement, suppression of parasitic absorption, and control of local overheating remain difficult.
Nanowires and nanotubes	3	3	3	Stability is moderate because one-dimensional structures can improve directional carrier transport but are sensitive to surface defects, contact degradation, and mechanical damage during assembly. Toxicity/safety is composition-dependent, ranging from relatively benign oxide nanowires to Cd-, Pb-, or chalcogenide-based systems with higher concern. Scalability is moderate because alignment, junction resistance, interfacial control, and uniform large-area integration remain challenging.
Two-dimensional materials and MXenes	3	4	3	Stability is moderate because graphene and transition-metal dichalcogenides can be robust, but MXenes are prone to oxidation, restacking, and surface-termination changes. The toxicity/safety score is comparatively favorable because many 2D materials avoid Pb/Cd chemistry, although solvent use, nanosheet inhalation risk, and environmental persistence still require assessment. Scalability is moderate because flake-size variability, dispersion control, film uniformity, and reproducible interfacial contact remain limiting.
Superlattices	3	3	2	Stability is moderate because periodic interfaces can effectively scatter phonons and modify electronic density of states, but repeated thermal cycling may cause interdiffusion, interface roughening, and strain-related degradation. Toxicity/safety is composition-dependent because many high-performance thermoelectric superlattices use Bi, sb, Te, pb, or related chalcogenides. Scalability is low because epitaxial or highly controlled deposition routes are costly, slow, and difficult to translate into large-area, mechanically robust modules.

(*Continued*)

TABLE 4 Continued

Nanomaterial platform	Stability score	Toxicity/Safety score	Scalability score	Basis for scoring and translational interpretation
Hierarchical nanocomposites	3	3	3	Stability is moderate because multiscale grains, nanoprecipitates, defects, and embedded phases improve phonon scattering but can also introduce phase segregation, interfacial degradation, and thermal-cycling fatigue. Toxicity/safety is moderate because performance may rely on Te-, Pb-, Sb-, or Se-containing thermoelectric chemistries. Scalability is moderate because powder processing and sintering are feasible, but reproducible phase distribution, contact durability, and module-level reliability remain difficult.
Nanostructured oxides and chalcogenides	4	3	4	Oxides receive a higher stability score because many show stronger resistance to heat, oxygen, and moisture than perovskites or quantum dots, while some chalcogenides are less stable depending on composition. Toxicity/safety is moderate because oxides are often comparatively safer, but sulfides, selenides, tellurides, and doped chalcogenides may introduce toxicity, scarcity, or environmental concerns. Scalability is relatively favorable because oxide and chalcogenide films, powders, and ceramics can be processed using established routes, although conductivity, dopant control, sintering reproducibility, and defect management remain limiting.
Carbon nanomaterials	4	4	3	Carbon nanomaterials score relatively well in stability because graphene, carbon nanotubes, and related carbon frameworks can provide chemical robustness, conductivity, and mechanical flexibility. Toxicity/safety is comparatively favorable because they avoid heavy-metal absorber chemistries, although inhalation risk, persistence, and occupational exposure still require control. Scalability is moderate because dispersion, aggregation, chirality or defect variability, film uniformity, and contact reproducibility remain persistent manufacturing challenges.
Hybrid PV–TEG nanostructures	2	3	2	The low stability score reflects coupled degradation under heat, illumination, humidity, electrical loading, thermal cycling, and interfacial stress. Toxicity/safety is moderate because the risk depends on the combined PV absorber, thermoelectric material, interconnect, encapsulant, and heat-transfer layer. Scalability is low because practical performance requires thermal matching, low contact resistance, reliable packaging, heat-sink integration, load matching, acceptable cost, and verified positive net power gain rather than simple addition of PV and TEG outputs.

charge extraction, direct residual heat, maintain thermoelectric gradients, and remain stable under realistic operating conditions. This concept is illustrated in Figure 5.

3.5 Translational barriers: the stability–toxicity–scalability trilemma

A persistent limitation in nano energy research is the gap between laboratory performance and deployable device value. Materials that show high photovoltaic efficiency, strong light absorption, improved thermoelectric figure of merit, or enhanced hybrid PV–TEG output are not necessarily suitable for large-scale energy systems (Shi et al., 2025). For interface-programmed nano energy platforms, translational viability is controlled by three linked constraints: stability, toxicity, and scalability. These constraints form a stability–toxicity–scalability trilemma because improving one dimension can expose weaknesses in the others. The semi-quantitative scoring matrix in Table 4 applies this trilemma directly to each nanomaterial platform by linking stability, toxicity/safety, and scalability scores to the dominant material-specific limitations

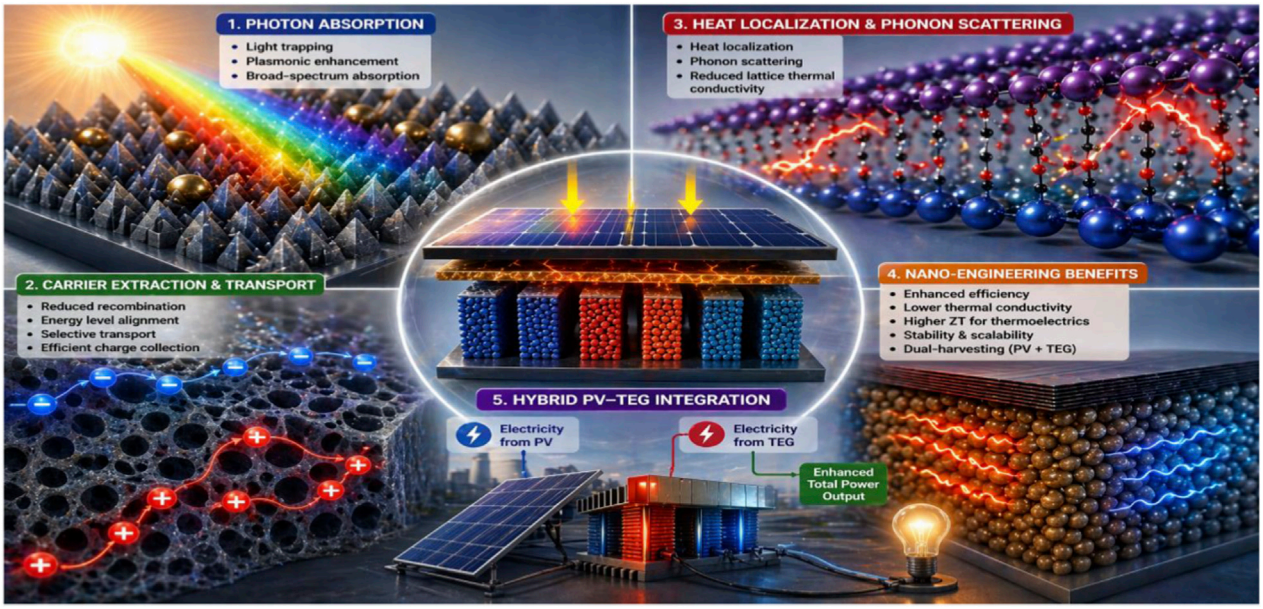


FIGURE 5
Conceptual framework of interface-programmed nano energy systems showing photon absorption, carrier extraction, heat localization, phonon scattering, and hybrid photovoltaic–thermoelectric integration.

identified in the reviewed solar, thermoelectric, and hybrid PV–TEG literature.

Stability determines whether a nano energy material can retain function under realistic operating stress. For photovoltaic nanomaterials, this includes resistance to moisture, oxygen, ultraviolet exposure, heat, illumination, electrical bias, and ion migration (Yan et al., 2020). For thermoelectric nanostructures, stability includes resistance to thermal cycling, phase segregation, oxidation, mechanical fatigue, contact degradation, and interfacial diffusion. For hybrid PV–TEG systems, stability is more demanding because the photovoltaic and thermoelectric components experience coupled optical, electrical, thermal, and mechanical stress within the same architecture.

Toxicity determines whether high-performing materials can be manufactured, operated, recycled, or disposed of safely. Lead-containing perovskites and lead chalcogenide quantum dots raise concerns about environmental leakage and end-of-life management. Cadmium-based quantum dots face similar restrictions despite strong optical performance (Chintada and Golla, 2025). Tellurium-containing thermoelectrics are constrained by scarcity and supply concerns, while lead telluride systems combine toxicity with high-temperature durability challenges. Even plasmonic systems based on gold and silver may face cost and resource limitations, whereas copper or aluminum plasmonic alternatives require careful oxidation control.

Scalability determines whether nanoscale performance can be transferred from small-area proof-of-concept devices to reproducible modules (Kim et al., 2026). Many nano energy materials perform well under tightly controlled laboratory conditions but suffer when processed over larger areas. Perovskite nanocrystals may lose uniformity through grain-boundary defects, ion migration, or coating instability. Quantum-dot films may suffer from ligand-removal inconsistency, cracking, aggregation, or poor charge percolation. Thermoelectric nanocomposites may show high performance in pellets but lose reliability at the module level due to contact resistance, thermal-expansion mismatch, or interfacial fatigue. Two-dimensional materials and MXenes often face restacking, oxidation, flake-size variability, and batch-to-batch inconsistency.

The trilemma is especially important for hybrid photovoltaic–thermoelectric systems because interface failure can erase apparent performance gains (Wang et al., 2025). A nanostructured photovoltaic layer may increase absorption but also generate excess heat or accelerate degradation. A thermoelectric layer may recover heat but also increase photovoltaic temperature if thermal gradients are poorly managed. A plasmonic coating may improve local field intensity but cause parasitic heating. A highly nanostructured thermoelectric may reduce lattice thermal conductivity but introduce unstable interfaces or weak mechanical contacts. Therefore, material selection must be evaluated at the level of coupled device operation, not isolated material performance.

Figure 6 illustrates that high laboratory performance becomes translationally meaningful only when three deployment requirements are addressed simultaneously: operational stability, material safety, and scalable fabrication. In nano-enabled photovoltaic, thermoelectric, and hybrid PV–TEG systems, high power conversion efficiency, strong optical absorption, enhanced carrier extraction, low lattice thermal conductivity, or improved ZT cannot alone establish practical relevance. These performance gains must be evaluated together with resistance to heat, illumination, humidity, oxygen, electrical bias, and thermal cycling; the use of toxic or critical elements such as Pb, Cd, Te, and noble metals; and the ability to fabricate reproducible large-area devices or modules at acceptable cost.

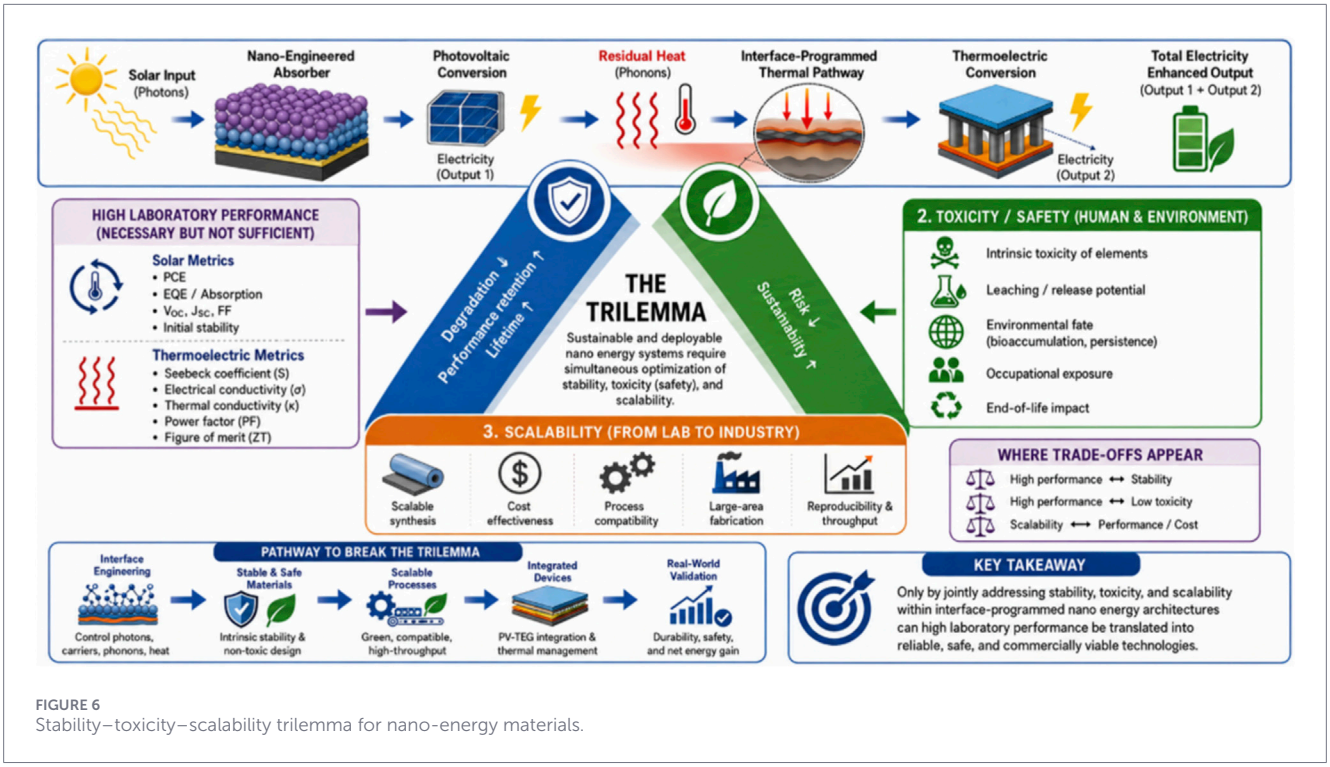


FIGURE 6
Stability–toxicity–scalability trilemma for nano-energy materials.

For future nano-energy studies, claims of application readiness should be supported by at least one clearly reported indicator from each arm of the trilemma. Stability evidence should include retained photovoltaic efficiency, thermoelectric power factor, ZT, or hybrid net power output after relevant stress testing, such as continuous illumination, heat-light-humidity exposure, electrical bias, thermal cycling, mechanical cycling, or long-term operation. Toxicity and sustainability evidence should include material composition, reduced use or replacement of Pb-, Cd-, Te-, or noble-metal-containing components, encapsulation or leakage-control strategy, solvent and processing burden, recyclability, occupational safety, and end-of-life management. Scalability evidence should include active device area, batch size, film or pellet uniformity, fabrication yield, processing temperature, module fabrication route, contact reproducibility, cost-relevant processing steps, and compatibility with solution processing, printing, sintering, roll-to-roll manufacturing, or other large-area fabrication pathways.

This trilemma reframes the evaluation of nano-energy systems from peak-performance reporting to deployment-oriented assessment. The most promising materials are therefore not necessarily those with the highest reported efficiency, absorption coefficient, Seebeck coefficient, power factor, or ZT, but those that retain adequate performance under realistic operating stress while reducing toxicity risks and enabling reproducible device fabrication. For example, perovskite nanocrystals and quantum dots require stronger evidence of long-term stability, ion-migration control, and reduced Pb/Cd risk; thermoelectric chalcogenides require attention to Te scarcity, contact durability, and module-level reliability; while hybrid PV–TEG systems must demonstrate net power gain after accounting for heat routing, PV temperature rise, contact resistance, packaging, heat-sink requirements, and load matching. In this sense, the stability–toxicity–scalability trilemma functions as a practical screening filter for identifying which nanomaterials can move from laboratory demonstrations toward interface-programmed solar, thermoelectric, and hybrid PV–TEG energy platforms.

3.6 Nano energy reporting and benchmarking framework

A major limitation across nano energy literature is the lack of standardized reporting, which makes it difficult to compare results across photovoltaic, thermoelectric, and hybrid PV–TEG studies (Ibrahim et al., 2025). Many reports emphasize peak efficiency, Seebeck coefficient, or isolated performance gains without providing sufficient detail on synthesis conditions, device architecture, stability, or system-level operation (Yousif and Jalil, 2024). As a result, improvements are often difficult to reproduce, interpret, or translate into deployable technologies.

To address this issue, a structured nano energy reporting and benchmarking framework in Table 5 is proposed. This framework is designed specifically for interface-programmed solar, thermoelectric, and hybrid systems, where performance depends on the coordinated behaviour of photons, carriers, phonons, and interfaces. The objective is to ensure that reported results are not only technically valid, but also comparable, reproducible, and relevant to device-level and system-level operation. The checklist emphasizes three principles. First, material properties must be reported in a way that allows independent reproduction. Second, device performance must be evaluated under clearly defined and realistic conditions. Third, claims of improvement must be supported by stability, sustainability, and scalability evidence. Without these elements, reported gains in efficiency or ZT cannot be reliably interpreted or compared.

TABLE 5 Reporting and benchmarking checklist for nano energy systems.

Domain	Minimum reporting requirement	Relevance to nano energy systems
Material identity	Composition, phase purity, morphology, size distribution, defect density, surface passivation strategy	Determines optical absorption, carrier transport, and interfacial behaviour
Synthesis and processing	Precursors, synthesis route, temperature, atmosphere, time, post-treatment, ligand or dopant control	Nano-scale properties are highly sensitive to synthesis conditions and affect reproducibility
Device architecture	Layer sequence, thickness, active area, contacts, encapsulation, measurement configuration	Governs interface quality, charge extraction, heat flow, and overall device performance
Solar performance metrics	PCE, J_{SC}, V_{OC}, fill factor, spectral response, active area, stability protocol	Prevents selective reporting of efficiency and ensures comparability across photovoltaic systems
Thermoelectric metrics	Seebeck coefficient, electrical conductivity, thermal conductivity, power factor, ZT, operating temperature range	Enables evaluation of coupled electrical and thermal transport
Hybrid PV–TEG metrics	PV-only output, TE-only output, integrated output, net hybrid gain, photovoltaic temperature, thermoelectric temperature gradient, load matching	Demonstrates whether hybridization produces a real system-level benefit
Stability assessment	Thermal cycling, illumination stability, humidity exposure, electrical bias, mechanical cycling, retention over time	Indicates whether performance is maintained under realistic operating conditions
Sustainability and toxicity	Presence of pb, Cd, Te, noble metals, solvent use, recyclability, environmental risk considerations	Determines environmental and regulatory feasibility
Scalability indicators	Active area, batch size, yield, uniformity, processing cost, compatibility with large-area or roll-to-roll fabrication	Distinguishes laboratory demonstrations from scalable technologies

This framework is intended to move nano energy research from isolated performance reporting toward mechanism-aware and application-relevant evaluation. For photovoltaic studies, reporting should extend beyond efficiency to include degradation pathways and interfacial stability. For thermoelectric studies, reporting should include temperature gradients, contact resistance, and module-level output. For hybrid PV–TEG systems, the key requirement is demonstration of net energy gain under controlled and comparable conditions, rather than additive reporting of photovoltaic and thermoelectric outputs. By standardizing how materials, devices, and systems are reported, this checklist supports more reliable comparison across studies and helps identify which nanomaterial strategies are genuinely suitable for integration into stable, scalable, and environmentally acceptable nano energy platforms.

4 Research gaps and future directions

Despite rapid progress in nano-enabled solar conversion, thermoelectric power generation, and hybrid PV–TEG systems, several unresolved gaps continue to limit mechanistic understanding and practical deployment. These gaps are not isolated rather are connected by the same central issue identified throughout this review as identified in Table 6: nano energy performance depends on coordinated control of photons, carriers, phonons, and interfaces. First, there is a mechanistic separation gap. Many studies report improved photovoltaic efficiency, enhanced thermoelectric performance, or increased hybrid output without clearly separating optical, electronic, thermal, and interfacial contributions. For example, an observed increase in photovoltaic current may result from improved absorption, reduced recombination, better charge extraction, or thermal artefacts. Similarly, improved thermoelectric performance may arise from phonon scattering, carrier filtering, contact effects, or measurement conditions. Future studies should therefore combine operando spectroscopy, thermal imaging, impedance analysis, carrier-lifetime measurements, and multiphysics modelling to identify the dominant mechanism responsible for performance gains.

Second, there is a benchmarking gap. Photovoltaic, thermoelectric, and hybrid PV–TEG studies often use different test conditions, device areas, temperature ranges, illumination intensities, heat-sink configurations, and reporting formats. This prevents direct comparison across studies and can exaggerate apparent progress. Hybrid systems are especially affected because added thermoelectric output is often reported without consistent comparison to PV-only and TEG-only baselines. Future work should adopt standardized reporting of active area, illumination condition, operating temperature, temperature gradient, load matching, contact resistance, and net system output.

Third, there is a coupled-stability gap. Most nano energy materials are tested under simplified stress conditions, yet real devices experience combined exposure to heat, light, oxygen, humidity, electrical bias, and thermal cycling. This is particularly important for perovskite nanostructures, quantum-dot films, plasmonic interfaces, flexible electrodes, and thermoelectric nanocomposites. Future studies should move from single-factor stability tests toward combined-stress protocols that report retention percentage, degradation pathway, failure mode, and recovery behaviour.

Fourth, there is a translation gap. Many high-performing nano energy materials depend on toxic elements, scarce resources,

TABLE 6 Gap-to-opportunity matrix for future nano energy research.

Research gap	Current limitation	Opportunity	Recommended research direction
Mechanistic separation	Performance gains are often reported without distinguishing optical absorption, carrier extraction, phonon scattering, thermal effects, and interfacial contributions	Build stronger causal evidence for nano-enabled performance	Use operando spectroscopy, thermal imaging, impedance analysis, carrier-lifetime measurements, and multiphysics simulation
Benchmarking inconsistency	Solar, thermoelectric, and hybrid PV–TEG studies use different device areas, operating temperatures, illumination conditions, and reporting formats	Improve comparability across material classes and device architectures	Report active area, illumination intensity, temperature gradient, heat-sink condition, load matching, contact resistance, and measurement configuration
PV–TEG net-gain uncertainty	Hybrid systems often report added TEG output without proving true integrated system benefit	Demonstrate real device-level advantage	Compare PV-only, TEG-only, and integrated PV–TEG output under identical conditions and report net gain after thermal and electrical losses
Stability under coupled stress	Heat, light, oxygen, humidity, bias, and mechanical cycling are often tested separately	Establish realistic operational durability	Conduct combined-stress testing with retention percentage, degradation pathway, and failure-mode analysis
Toxicity and critical-material dependence	High-performing systems may rely on pb, Cd, Te, rare elements, noble metals, or solvent-intensive processing	Improve environmental acceptability and deployment feasibility	Develop lead-reduced or lead-free perovskites, heavy-metal-free quantum dots, earth-abundant thermoelectrics, recyclable architectures, and safer processing routes
Scalable fabrication	Many nanomaterials perform well only in small-area laboratory devices	Move from proof-of-concept demonstrations to reproducible modules	Report batch size, active area, yield, film uniformity, processing cost, roll-to-roll compatibility, and module-level validation
Interface durability	Interfaces may degrade through diffusion, oxidation, delamination, thermal-expansion mismatch, or contact resistance growth	Strengthen the interface-programmed design framework	Develop chemically stable interlayers, compliant thermal contacts, encapsulation strategies, and accelerated cycling protocols
System-level integration	Device studies often optimize materials without considering packaging, heat management, mass, and cost	Improve practical hybrid PV–TEG design	Couple materials discovery with thermal modelling, packaging design, life-cycle assessment, and techno-economic analysis

unstable interfaces, or processing routes that are difficult to scale. Lead- and cadmium-based absorbers, tellurium-containing thermoelectrics, noble-metal plasmonic structures, and solvent-intensive nanomaterial processing all raise concerns for deployment. Future research should prioritize lead-reduced or lead-free perovskites, heavy-metal-free quantum dots, earth-abundant thermoelectrics, oxidation-resistant two-dimensional materials, recyclable device structures, and lower-toxicity processing routes.

Fifth, there is a hybrid-system validation gap. PV–TEG studies frequently report gross output rather than true net gain after considering thermal losses, added resistance, temperature rise in the photovoltaic layer, additional mass, heat-sink requirements, packaging complexity, and cost. A hybrid system should only be considered beneficial if the integrated architecture outperforms the photovoltaic-only and thermoelectric-only references under identical conditions. Future PV–TEG studies should therefore report net power gain, photovoltaic temperature, thermoelectric temperature difference, load-matching strategy, contact resistance, stability under thermal cycling, and device-level energy balance.

Recent PV–TEG demonstrations also clarify how this translational roadmap should evolve from conceptual hybridization toward deployable interface-engineered systems. Monolithic PV–TEG devices using exothermic reactive interlayers show that thermal interface engineering can reduce coupling losses and improve heat transfer between the photovoltaic and thermoelectric stages (Kim et al., 2019). Unified dye-sensitized solar cell–thermoelectric architectures based on bipolar conduction indicate that future hybrid systems may

benefit from shared or multifunctional elements rather than mechanically stacked subdevices (Kim et al., 2020). Bandgap-engineered metal oxides and black TiO_2 photothermal materials further demonstrate that absorber chemistry and photothermal conversion layers can be tuned to enhance solar absorption, heat localization, and thermoelectric temperature-gradient generation (Parkavi et al., 2026; Parkavi et al., 2025). Flexible PIN-type photo-thermoelectric configurations extend this direction toward lightweight, bendable, and potentially wearable or building-integrated energy harvesters (Prabhu et al., 2026). Future PV–TEG deployment should therefore prioritize low-resistance thermal contacts, spectrally selective and thermally stable photothermal materials, mechanically compliant interlayers, flexible module architectures, and standardized testing against PV-only and TEG-only baselines under matched illumination, temperature, heat-sink, device-area, and load-matching conditions.

Future research should therefore shift from isolated material optimization toward integrated, mechanism-aware device validation. Machine-learning-guided materials discovery, high-throughput synthesis, operando characterization, multiphysics simulation, life-cycle assessment, and techno-economic analysis should be used together rather than separately. For solar conversion, priority should be given to stable perovskite interfaces, heavy-metal-free quantum dots, spectrally selective absorbers, and durable transport layers. For thermoelectrics, emphasis should be placed on mechanically robust nanocomposites, earth-abundant compositions, low-contact-resistance modules, and thermal-cycling durability. For hybrid PV–TEG systems, the decisive research direction is clear: demonstrate reproducible net energy gain under realistic operating conditions while maintaining stability, material safety, and scalable fabrication.

5 Conclusion

This critical mini-review shows that the future value of nano-enabled solar, thermoelectric, and hybrid PV–TEG systems will depend less on isolated material performance and more on how interfaces coordinate photon absorption, charge extraction, phonon transport, heat routing, and device stability. The central message is that high photovoltaic efficiency, strong optical absorption, high power factor, or improved ZT cannot by themselves confirm practical relevance. These metrics become meaningful only when they are supported by stable operation, low toxicity risk, scalable fabrication, reliable contacts, and verified net system-level energy gain. The interface-programmed nano-energy framework developed in this review provides a practical way to connect nanoscale mechanisms with deployable energy technologies. For solar materials, the priority is to enhance light absorption and carrier extraction without increasing recombination, parasitic heating, heavy-metal risk, or environmental instability. For thermoelectric materials, the key challenge is to reduce lattice thermal conductivity through phonon scattering while preserving carrier mobility, contact durability, and thermal-cycling reliability. For hybrid PV–TEG systems, the decisive requirement is not simple device stacking but controlled thermal coupling, photovoltaic temperature management, preservation of the TEG temperature gradient, electrical load matching, and demonstration of true net power gain under matched operating conditions. This review also highlights the stability–toxicity–scalability trilemma as a critical filter for identifying which nanomaterials can move beyond laboratory demonstrations. Quantum dots, perovskite nanocrystals, plasmonic nanoparticles, hierarchical thermoelectric composites, two-dimensional materials, and hybrid PV–TEG architectures all offer important performance opportunities, but each faces specific barriers related to degradation, Pb/Cd/Te or noble-metal dependence, interfacial failure, reproducibility, or large-area processing. Therefore, future nano-energy studies should report not only efficiency or ZT, but also active area, device architecture, contact resistance, operating temperature, thermal gradient, stability retention, toxicity/sustainability evidence, fabrication route, and scalability indicators. Overall, this review provides researchers, materials scientists, device engineers, and energy-system designers with a clearer roadmap for translating nano-energy concepts into practical technologies. Progress in the field will require a shift from performance-driven material optimization toward mechanism-aware, interface-programmed, and deployment-oriented design. The most promising future systems will be those that combine efficient solar conversion, useful waste-heat recovery, durable interfaces, safer material chemistry, scalable processing, and validated net energy benefit. Such an approach can improve the visibility and practical relevance of nano-energy research for readers interested in advanced photovoltaics, thermoelectrics, hybrid energy harvesting, and sustainable energy technologies.

Author contributions

VE: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review and editing.

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