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Artificial Intelligence as a Convergence Catalyst in the Physical and Chemical Sciences: Advances in Materials Discovery, Nanostructured Energy Storage, and Space Weather Physics

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Abstract

Background: Artificial intelligence (AI) and machine learning (ML) are increasingly used as general-purpose research instruments across the physical sciences, accelerating tasks that were traditionally limited by trial-and-error experimentation, computational cost, or the sheer dimensionality of the underlying physics. Three areas illustrate this shift with particular clarity: computational materials discovery, nanostructured electrode design for energy storage, and space weather / heliophysics forecasting. Despite substantial progress in each area individually, limited work has examined them together, quantitatively, as expressions of a single underlying trend — the convergence of AI methodology with core physical and chemical science. Methods: This study used a narrative and scoping review methodology, incorporating quantitative benchmarks drawn directly from primary and independent critical sources. Peer-reviewed literature, preprints, direct observational monitoring data, and ResearchGate-hosted scholarly works published primarily between 2023 and 2026 were identified through structured searches combining terms from materials informatics, nanostructured energy-storage materials, and AI-based space weather forecasting. Sources were screened for topical relevance and synthesized thematically, with reported quantitative claims cross-checked against independent critical appraisal where available. Results: The synthesis identifies convergent innovation across three domains, with all three now quantitatively documented: (1) AI-driven inverse design (exemplified by a 2.2-million-structure materials search yielding roughly 380,000 candidate stable materials) is accelerating materials discovery, though independent re-analysis found only a small fraction of these structures met joint criteria of novelty, credibility, and utility; (2) nanostructured graphene–metal oxide composite electrodes span a wide reported performance envelope (specific capacitances from roughly 100 F/g to over 1000 F/g; energy densities up to roughly 100+ Wh/kg), with statistically designed synthesis optimization improving reproducibility; and (3) AI-assisted forecasting achieved approximately one-minute precision in reconstructing a major 2024 geomagnetic superstorm, in contrast to a roughly 40% amplitude error and nine-month timing error in the leading pre-cycle statistical/physical forecast of Solar Cycle 25's overall intensity. Discussion: A common methodological pattern recurs across all three domains: AI is used not to replace physical theory but to navigate high-dimensional parameter spaces that are analytically or computationally intractable by classical means alone, and the strongest, most defensible results are those subjected to independent, domain-expert critical appraisal rather than accepted at face value. Conclusion: Continued progress will depend on higher-quality shared datasets, physics-informed model architectures, standardized benchmarking protocols, and routine independent critical appraisal as a formal part of the AI-for-science publication cycle.

Keywords: artificial intelligence; materials discovery; inverse design; nanostructured electrodes; graphene–metal oxide composites; supercapacitors; space weather forecasting; geomagnetic storms; interdisciplinary science

1. Introduction

The physical and chemical sciences have historically advanced through a cycle of theory, experiment, and, since the mid-twentieth century, numerical simulation. Artificial intelligence is now widely described as a fourth pillar of this cycle, particularly where the underlying design or parameter space is too large to search exhaustively by classical computational or experimental means (Cheng, Fu, Okabe, et al., 2026). Materials science, energy-storage engineering, and space weather physics are three domains in which this shift is especially visible, and in which AI methods are being adopted not as peripheral analytic tools but as core components of the discovery and forecasting pipeline.

In materials science, AI-driven inverse design allows researchers to specify a desired material property and generate candidate structures algorithmically, reversing the traditional forward-screening paradigm in which candidate materials are proposed first and their properties computed afterward (Cheng et al., 2026). Related applied scholarship frames this as a broader convergence of chemistry, physics, and artificial intelligence, in which data-driven methods increasingly sit alongside — rather than beneath — first-principles and experimental approaches to material design (Mishra, Mishra, & Agarwal, 2025a, 2024).

In energy-storage engineering, nanostructured graphene–metal oxide composite electrodes have emerged as a leading architecture for supercapacitors, combining the high electrical conductivity and mechanical stability of graphene-based scaffolds with the high specific capacitance of transition-metal oxides (Mishra, Mishra, & Agarwal, 2025b). Because electrode performance depends on a large number of interacting structural and electrochemical parameters, optimizing these composites is itself increasingly treated as a data-driven design problem rather than a purely empirical one.

In space weather physics, deep learning and hybrid physics–machine-learning models are being applied to forecast solar flares, coronal mass ejections (CMEs), and their downstream geomagnetic effects, with recent work demonstrating that AI methods could, in principle, have anticipated the full causal chain of events associated with major recent superstorms (Guastavino, Legnaro, Massone, & Piana, 2025). This work has taken on additional urgency during Solar Cycle 25, which has proven markedly more active than pre-cycle predictions anticipated (Mishra, Mishra, & Agarwal, 2026a, 2026b; Agarwal, Mishra, & Mishra, 2026).

The objective of this review is to synthesize innovative AI-related research across these three domains and to characterize the methodological pattern that connects them. Specifically, the review addresses three questions: (a) What are the principal AI-driven innovations reported in materials discovery, nanostructured energy-storage design, and space weather forecasting between approximately 2024 and 2026? (b) What common methodological logic, if any, underlies AI's role across these otherwise distinct physical and chemical domains? and (c) What limitations and evaluation challenges are shared across these applications? Table 1 summarizes the scope of the three domains as treated in this review.

Table 1. Scope of the three reviewed domains.

Domain	Core Question	Primary Methods Represented
AI-Driven Materials Discovery	Can AI navigate the space of candidate materials faster and more precisely than forward screening?	Inverse design, generative models, deep-learning property prediction, reinforcement learning
Nanostructured Energy Storage	How can electrode nanostructure be optimized for energy density, power density, and cycle life?	Graphene–metal oxide composite design, data-driven electrochemical optimization
Space Weather & Heliophysics Forecasting	Can AI improve the lead time and accuracy of solar-terrestrial event forecasting?	Deep learning (CNN/LSTM/Vision Transformer), hybrid physics–ML models, ensemble forecasting

2. Materials and Methods

2.1. Review Design

This study used a narrative and scoping review design rather than a formal systematic review with meta-analysis, reflecting both the breadth of the three domains under consideration and the heterogeneity of evidence types available — ranging from computational benchmarking studies to applied engineering reviews. Scoping methodology is appropriate for mapping the breadth of a fast-moving, cross-disciplinary literature and for identifying recurring methodological patterns rather than pooling quantitative effect sizes.

2.2. Search Strategy and Sources

A structured search was conducted across peer-reviewed journals, preprint servers (including arXiv), and scholarly works hosted on ResearchGate. Search terms were grouped into three thematic clusters and combined using Boolean operators:

- Cluster 1 (Materials): "artificial intelligence materials discovery," "inverse design," "generative models materials," "machine learning materials design"
- Cluster 2 (Energy storage): "graphene metal oxide composite," "nanostructured electrode," "supercapacitor optimization," "energy density power density cycling stability"
- Cluster 3 (Space weather): "AI space weather forecasting," "geomagnetic storm machine learning," "solar flare deep learning," "coronal mass ejection prediction," "Solar Cycle 25"

Searches were restricted primarily to literature published between 2024 and 2026 to capture the most recent wave of innovation. Where a specific author's applied scholarship on a topic (e.g., materials–AI convergence, or space weather physics during Solar Cycle 25) was identified as directly relevant, it was included and is flagged in the Results as such; because these works are hosted on the ResearchGate platform rather than indexed by a conventional publisher database, independent verification of the exact publication venue was not always possible, and this limitation is noted explicitly in Section 4.5.

2.3. Screening and Inclusion Criteria

Sources were included if they (a) reported original research, a review, or a substantive applied analysis; (b) addressed at least one of the three thematic clusters; and (c) were attributable to an identifiable author or institutional source. Sources were excluded if they were purely promotional or lacked identifiable authorship. No formal risk-of-bias scoring was applied, consistent with standard scoping-review practice; instead, each source was evaluated qualitatively for methodological transparency (e.g., stated datasets, benchmarks, or theoretical derivations), and claims are described as theoretical, simulation-based, or empirically validated where the distinction is material to interpretation.

2.4. Data Synthesis

Extracted information was organized thematically according to the three-domain structure in Table 1. For each domain, the synthesis captured the principal technical innovation reported, the methodological approach used to demonstrate it, reported outcomes, and explicitly acknowledged limitations. Cross-cutting methodological patterns — particularly the recurring use of AI to navigate high-dimensional design or forecasting spaces — were identified through iterative comparison across the three thematic sets.

3. Results

3.1. AI-Driven Materials Discovery and Design

The reviewed literature describes a paradigm shift in computational materials science from forward screening — in which candidate materials are proposed and their properties subsequently computed or measured — toward inverse design, in which a target property is specified and candidate structures are generated algorithmically. This shift spans high-throughput forward machine-learning methods and evolutionary algorithms through to deep generative models and reinforcement learning, with recent large-language-model-based systems now capable of proposing stable inorganic crystal structures or metal–organic frameworks directly from textual property specifications (Cheng et al., 2026).

Applied scholarship situates this technical trajectory within a broader convergence narrative, arguing that materials science is increasingly defined by the integration of chemistry, physics, and artificial intelligence into a single data-driven, predictive research paradigm, in which computational modeling and machine learning augment — rather than simply accelerate — traditional experimental methodology (Mishra, Mishra, & Agarwal, 2025a). Related applied work frames AI-powered material design specifically as a response to the practical limitations of conventional trial-and-error approaches, which face compounding constraints as the complexity of target chemical compositions, structures, and desired properties increases (Mishra, Mishra, & Agarwal, 2024).

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The most widely cited empirical demonstration of AI-driven materials discovery to date is Graph Networks for Materials Exploration (GNoME), a graph-neural-network system trained at scale on the Materials Project and Open Quantum Materials Database. GNoME generated 2.2 million candidate crystal structures, of which approximately 381,000 were predicted to be thermodynamically stable, expanding the number of known stable inorganic materials from roughly 48,000 to approximately 421,000 — an order-of-magnitude increase that the original authors described as equivalent to nearly 800 years of conventional discovery effort (Merchant, Batzner, Schoenholz, Aykol, Cheon, & Cubuk, 2023). This result is frequently cited in the applied literature as headline evidence of AI's transformative potential for materials science.

However, subsequent independent scrutiny of these claims illustrates the importance of rigorous post-hoc evaluation of AI-generated scientific output. A detailed materials-chemistry perspective on the GNoME dataset concluded that, on close inspection, only a small fraction of the reported structures satisfied the joint criteria of genuine novelty, chemical credibility, and practical utility, with many entries duplicating known compounds, containing implausible coordination environments, or lacking any clear synthetic pathway (Cheetham & Seshadri, 2024). A separate investigation reported in the trade press subsequently identified extensive near-duplicate structures within the GNoME dataset and called for correction of the associated publication record, noting that the issue had accumulated roughly a thousand citations before being widely flagged (Chemical & Engineering News, 2025). Table 2 summarizes the headline GNoME claims alongside this subsequent critical appraisal.

Table 2. AI-driven materials discovery: Headline claims versus subsequent critical appraisal (GNoME case study).

Metric / Claim	Reported Value	Source
Candidate crystal structures generated	2.2 million	Merchant et al. (2023)
Structures predicted thermodynamically stable	~381,000 (~421,000 stable materials known in total, up from ~48,000)	Merchant et al. (2023)
Claimed discovery-efficiency gain	"Order-of-magnitude expansion"; equivalent to ~800 years of prior discovery effort	Merchant et al. (2023)
Independent re-assessment of novelty/credibility/utility	"Scant evidence" that most structures meet all three criteria jointly	Cheetham & Seshadri (2024)
Duplicate/near-duplicate structure concerns	Extensive duplication identified; correction/retraction discussion initiated	Chemical & Engineering News (2025)

3.2. Nanostructured Graphene–Metal Oxide Composites for Energy Storage

A second domain of innovation concerns the design of nanostructured electrode materials for supercapacitors. Graphene-based scaffolds combined with transition-metal oxides are widely reported to produce a synergistic effect: the graphene component contributes high electrical conductivity and mechanical/structural stability, while the metal oxide component contributes high specific capacitance through reversible redox reactions at the electrode surface. Applied engineering scholarship on this architecture reports design and optimization strategies aimed at simultaneously improving energy density, power density, and long-term cycling stability — three properties that are often in tension with one another in conventional electrode designs (Mishra, Mishra, & Agarwal, 2025b). Table 3 summarizes the principal design trade-offs and reported mitigation strategies identified in the reviewed literature.

Table 3. Design trade-offs in nanostructured graphene–metal oxide supercapacitor electrodes.

Performance Property	Limiting Factor	Reported Mitigation Strategy
Energy density	Limited redox-active surface area in bulk metal oxides	Nanostructuring of metal oxide phase to increase accessible surface area
Power density	Poor intrinsic electrical conductivity of metal oxides	Hybridization with conductive graphene / reduced graphene oxide scaffold
Cycling stability	Structural degradation of metal oxide phase under repeated charge/discharge	Graphene matrix acts as a mechanical buffer, limiting structural fatigue
Rate capability	Slow ion diffusion through dense composite structures	Porous, 3D-structured composite architectures to shorten ion diffusion paths

Because electrode performance depends on a large number of interacting variables — nanostructure morphology, metal oxide loading, synthesis temperature, and electrolyte composition, among others — this literature increasingly treats electrode optimization as a structured design-space search problem, conceptually parallel to the inverse-design methods described in Section 3.1, even where the specific studies do not themselves apply machine learning directly to the electrode optimization task.

Representative quantitative benchmarks illustrate both the promise and the variability of this design space. A design-of-experiments-optimized three-dimensional reduced-graphene-oxide (rGO) aerogel, produced via hydrothermal reduction with synthesis parameters tuned using a Taguchi statistical design, achieved a maximum specific capacitance of 182.33 F/g at 0.2 A/g, corresponding to an energy density of 6.33 Wh/kg at a power density of 108.5 W/kg in aqueous KOH electrolyte (Abdou Ahmed Abdou Elsehsah, Ahmad Noorden, Mat Saman, et al., 2025). This result illustrates that even without metal oxide hybridization, systematic, statistically designed optimization of synthesis parameters can meaningfully improve reproducibility and performance relative to ad hoc synthesis protocols. A comprehensive review of graphene-based metal oxide composites more broadly reports that hybridization with pseudocapacitive metal oxides — including MnO_2, Co_3O_4, NiO, and RuO_2 — can substantially exceed the specific capacitance achievable with graphene alone, with the review's surveyed literature spanning specific capacitances from roughly 100 F/g up to values exceeding 1000 F/g depending on metal oxide loading, morphology, and hybridization strategy, alongside corresponding gains in energy density where nanostructuring successfully increases redox-active surface area (Yallur, Rao, Harshitha, et al., 2025). Table 4 situates these benchmarks within the broader reported performance envelope for graphene–metal oxide and related graphene-based composite electrodes.

Table 4. Representative quantitative performance benchmarks for graphene-based supercapacitor electrodes.

Electrode System	Specific Capacitance	Energy Density (Power Density)	Cycling Retention	Source
Taguchi-optimized 3D rGO aerogel (no metal oxide)	182.33 F/g @ 0.2 A/g	6.33 Wh/kg (108.5 W/kg)	Not reported	Abdou Ahmed Abdou Elsehsah et al. (2025)
Graphene–metal oxide composites (surveyed range)	~100 F/g to >1000 F/g, depending on oxide/loading	Up to ~100+ Wh/kg in optimized architectures	Frequently >70–90% after 5,000–10,000 cycles across surveyed studies	Yallur, Rao, Harshitha, et al. (2025), review synthesis
Graphene–metal oxide composite electrodes (applied design study)	Reported as substantially improved vs. unhybridized graphene	Reported gains in both energy and power density	Cycling stability specifically targeted as a design objective	Mishra, Mishra, & Agarwal (2025b)

Taken together, these benchmarks indicate that the reported performance envelope for graphene–metal oxide composites is wide, reflecting the strong sensitivity of electrochemical performance to nanostructure design choices. This variability itself supports the case for more systematic, data-driven optimization approaches: the roughly order-of-magnitude spread in specific capacitance values across the reviewed literature (from approximately 100 F/g to over 1000 F/g) suggests a design space large enough that manual, single-variable-at-a-time experimentation is unlikely to efficiently locate optimal configurations, paralleling the motivation for inverse-design methods in Section 3.1.

3.3. Artificial Intelligence in Space Weather and Heliophysics Forecasting

The third domain concerns the application of AI to forecasting solar and geomagnetic activity. A representative empirical demonstration applied AI methods to reconstruct the full causal chain of the May 2024 superstorm — from solar flare onset through CME propagation to the resulting geomagnetic storm — using a Vision Transformer for active-region morphology classification, a video-based deep-learning model for flare-occurrence prediction, a physics-informed model for CME travel-time estimation, and a data-driven alerting model based on in-situ solar wind measurements; the combined system achieved CME arrival-time predictions accurate to within approximately one minute of uncertainty and outperformed traditional forecasting methods across the full event chain (Guastavino et al., 2025).

This body of work has particular relevance during Solar Cycle 25, which reviewed sources describe as substantially more energetically active than pre-cycle predictions anticipated, producing an unusually dense sequence of ground-level enhancements, Forbush decreases, and high-energy cosmic-ray modulation events (Mishra, Mishra, & Agarwal, 2026b; Agarwal, Mishra, & Mishra, 2026). This claim is independently corroborated by direct solar-cycle monitoring data: the 2019 international Solar Cycle 25 Prediction Panel forecast a smoothed peak sunspot number of 115 (uncertainty range 105–125), expected around July 2025, whereas the cycle's smoothed sunspot number actually peaked at approximately 160.8 in October 2024 — roughly 40% above the panel's upper bound and about nine months earlier than the central forecast date (Solar Influences Data Analysis Center [SIDC], 2024; NOAA Space Weather Prediction Center, 2023). This substantial and directionally consistent forecast error across multiple independent prediction methods illustrates the practical difficulty of long-lead-time heliophysical forecasting even using established statistical and physical modeling techniques, and helps explain the growing interest in AI-based approaches as a complementary forecasting tool. Complementary applied work specifically addresses AI-based real-time space weather prediction and geomagnetic storm forecasting as a practical operational challenge in this context (Mishra, Mishra, & Agarwal, 2026a). Table 5 juxtaposes the pre-cycle panel forecast against the observed outcome.

Table 5. Solar Cycle 25: Pre-cycle statistical/physical forecast versus observed outcome.

Quantity	Pre-Cycle Forecast (2019 Panel)	Observed Outcome	Source
Smoothed peak sunspot number	115 (range: 105–125)	≈160.8	NOAA SWPC (2023); SIDC (2024)
Expected timing of peak	July 2025 (± 8 months)	October 2024 (smoothed peak)	NOAA SWPC (2023); SIDC (2024)
Forecast error (peak amplitude)	—	≈+40% relative to panel's upper bound	Derived from SIDC (2024) and NOAA SWPC (2023)
CME arrival-time uncertainty (AI-assisted pipeline, May 2024 superstorm case)	N/A (retrospective AI demonstration)	≈1 minute uncertainty, outperforming classical forecasting methods	Guastavino, Legnaro, Massone, & Piana (2025)

This juxtaposition illustrates why AI-based forecasting methods are of particular practical interest in heliophysics: classical statistical and physics-based precursor methods, even when produced by an international expert panel synthesizing multiple independent techniques, substantially underestimated both the amplitude and mistimed the peak of Solar Cycle 25, whereas the AI-assisted pipeline evaluated retrospectively against the May 2024 superstorm achieved minute-level precision in CME arrival-time prediction — a qualitatively different order of forecasting precision, albeit for a shorter-horizon, event-specific prediction task rather than a multi-year cycle-amplitude forecast. The two forecasting problems are not directly comparable in difficulty, but the contrast is nonetheless informative about where AI methods currently add the most practical forecasting value.

Across the broader forecasting literature, tree-based methods (e.g., random forest, gradient boosting) are reported to perform well for short-term geomagnetic forecasts, while deep-learning approaches — particularly convolutional and recurrent architectures — offer superior performance for image-based and temporal prediction tasks, with hybrid architectures increasingly favored for real-time operational forecasting. Table 6 summarizes representative AI forecasting approaches by space weather event type.

Table 6. Representative AI forecasting approaches by space weather event type.

Event Type	Representative AI Approach	Reported Strength
Solar flare occurrence/onset	Vision Transformer / video-based deep learning on magnetogram data	Captures evolving active-region morphology prior to eruption (Guastavino et al., 2025)
CME propagation / arrival time	Physics-informed deep learning using coronal and solar-wind observations	Substantially reduced arrival-time uncertainty relative to classical models
Geomagnetic storm onset	Data-driven alerting models on in-situ solar wind measurements; LSTM/hybrid models	Improved short-lead-time warning accuracy; extended-lead-time variants in development
Cosmic ray modulation / GLEs	Statistical and ML-assisted multi-instrument analysis	Systematic characterization of Forbush decreases and ground-level enhancements across Solar Cycle 25 (Agarwal et al., 2026)

4. Discussion

4.1. A Shared Methodological Pattern

Across all three domains, AI is applied to the same underlying structural problem: navigating a high-dimensional space — of candidate chemical compositions, electrode nanostructure configurations, or solar-terrestrial physical states — that is too large or too computationally expensive to search exhaustively using classical forward methods alone. In materials discovery, this manifests as inverse design across a compositional space of GNoME's scale (2.2 million candidate structures, Table 2); in energy storage, as data-driven optimization across a design space wide enough to produce an order-of-magnitude spread in reported specific capacitance values, from roughly 100 F/g to over 1000 F/g across the surveyed literature (Table 4); and in space weather forecasting, as pattern recognition across high-dimensional, multi-instrument observational data spanning magnetogram imagery, coronal observations, and in-situ solar-wind measurements (Table 6). This structural similarity suggests that methodological advances in one domain — for example, generative modeling techniques originally developed for materials discovery — may plausibly transfer to related design or forecasting problems in the other domains, although the reviewed literature does not yet report direct cross-domain methodological transfer studies, and this transfer potential should accordingly be treated as a plausible hypothesis for future work rather than an established finding.

4.2. AI as a Complement to, Not a Replacement for, Physical Theory

A recurring pattern across the reviewed literature is that AI methods are most effective, and most trusted, when integrated with rather than substituted for physical theory. Physics-informed models for CME travel-time prediction outperform purely data-driven alternatives by explicitly incorporating known solar-wind physics, achieving approximately one-minute arrival-time uncertainty in the May 2024 superstorm case study (Guastavino et al., 2025; Table 5), a level of precision considerably beyond what purely statistical cycle-amplitude forecasts achieved for Solar Cycle 25 as a whole (Table 5). Applied materials-science scholarship similarly frames AI as augmenting first-principles and experimental methodology rather than superseding it (Mishra et al., 2025a), and the GNoME case study reinforces this point from the opposite direction: the components of the GNoME pipeline that relied on established physical criteria — high-throughput density-functional-theory stability calculations — were not themselves challenged by subsequent critique; rather, the critique concerned the interpretive leap from computed stability to genuine chemical novelty and synthesizability, a judgment that still depends on domain expertise and physical/chemical reasoning that the model itself does not supply (Cheetham & Seshadri, 2024). Taken together, this pattern echoes broader trends in AI-for-science scholarship and suggests that the most durable near-term applications of AI in the physical sciences are hybrid, physics-constrained architectures in which AI narrows a search space and physical theory or experiment adjudicates the result, rather than fully autonomous, end-to-end data-driven pipelines.

4.3. Interdisciplinary Dependencies

Each of the three domains reviewed also depends on interdisciplinary integration that extends beyond AI methodology narrowly construed. Materials discovery increasingly requires collaboration between computer scientists, chemists, and condensed-matter physicists — a dependency made explicit by the fact that GNoME's core technical contribution (graph-neural-network scaling) required chemistry-trained reviewers to properly evaluate its chemical outputs, a step that appears to have been comparatively underweighted in the initial publication relative to the computational contribution (Cheetham & Seshadri, 2024). Energy-storage electrode design bridges materials chemistry and electrochemical engineering, and increasingly statistics and experimental-design methodology, as illustrated by the Taguchi-designed optimization approach applied to rGO aerogel synthesis (Abdou Ahmed Abdou Elsehsah et al., 2025). Space weather forecasting bridges solar physics, geomagnetism, and machine learning, and — as the Solar Cycle 25 forecast error illustrates (Table 5) — even a well-resourced, internationally coordinated expert panel drawing on multiple independent physical and statistical models can substantially misjudge a slow, large-scale physical process, suggesting that interdisciplinary breadth alone does not guarantee forecasting accuracy without continual empirical recalibration. This mirrors patterns documented in the broader interdisciplinary-methodology literature, which argues that AI's inherently cross-disciplinary nature tends to catalyze methodological convergence across otherwise distinct scientific fields rather than functioning as a self-contained subfield of computer science.

4.4. Evaluation and Benchmarking Challenges

A common limitation across all three domains is the difficulty of benchmarking AI methods against strong physics-based baselines under realistic, operationally relevant conditions. In materials discovery, generated candidate structures require experimental validation before their practical utility can be confirmed, and the GNoME case demonstrates that headline scale metrics (2.2 million structures) can substantially overstate practically useful output if novelty, credibility, and synthesizability are not jointly and independently verified (Cheetham & Seshadri, 2024). In energy-storage design, laboratory-scale performance gains — such as the specific capacitance and energy density values summarized in Table 4 — do not always translate to manufacturable, large-scale devices, and reported performance envelopes vary by roughly an order of magnitude across studies, complicating direct comparison without standardized testing protocols (electrolyte, current density, and cell configuration all affect reported values). In space weather forecasting, models validated on a small number of well-documented historical events, such as the May 2024 superstorm, may not generalize reliably to the full diversity of solar-terrestrial disturbance types, and the substantial forecast error observed for Solar Cycle 25's overall amplitude (Table 5) is a reminder that even mature, decades-refined forecasting methodologies can be wrong by a wide margin at longer time horizons. Rigorous, standardized benchmarking — ideally against both classical physics-based methods and independent experimental or observational ground truth — remains an open methodological need across all three domains.

4.5. The Evaluation Gap: Critical Appraisal of AI-Generated Scientific Claims

The GNoME case study (Table 2) merits discussion as a distinct methodological lesson for AI-driven physical science more broadly, beyond its specific relevance to materials discovery. The original claims — 2.2 million new crystal structures, an order-of-magnitude expansion in known stable materials — were widely reported and cited (accumulating roughly a thousand citations within about two years) before a detailed independent chemistry-led re-analysis concluded that only a small fraction of the reported structures satisfied the joint criteria of novelty, credibility, and utility that would be required for the results to represent genuine, actionable materials discoveries (Cheetham & Seshadri, 2024). A subsequent trade-press investigation identified extensive near-duplicate structures within the released dataset, prompting renewed calls for correction of the scientific record (Chemical & Engineering News, 2025).

This sequence of events — headline claim, broad citation and uptake, and delayed independent scrutiny — illustrates a general evaluation gap that appears likely to recur across AI-for-science domains as publication and citation velocity in this area continues to outpace the domain-specific expert review needed to validate AI-generated outputs. The lesson generalizes beyond materials science: in energy-storage research, the wide spread of reported specific capacitance values (Table 4) similarly calls for caution in comparing headline performance numbers across studies that may differ in testing protocol, and in space weather forecasting, the strong performance of AI methods on a small number of well-studied benchmark events (Table 5) should not be assumed to generalize until tested against a broader and more heterogeneous event set. Readers and practitioners engaging with AI-for-science claims across all three domains reviewed here should therefore treat scale- or headline-based claims (e.g., number of structures generated, peak reported capacitance, minute-level forecast precision on a single case study) as provisional pending independent, domain-expert validation, rather than as settled scientific fact.

4.6. Limitations

This review has several limitations. First, as a narrative and scoping synthesis, it does not provide pooled quantitative estimates of effect and is subject to the selection considerations inherent in any thematic literature synthesis. Second, several applied sources relevant to materials-AI convergence and Solar Cycle 25 space weather physics are hosted on the ResearchGate platform; while such sources were screened for topical relevance and internal coherence, their exact publication venue, peer-review status, and priority relative to conventionally indexed literature could not always be independently verified, and readers relying on this review for citation purposes in a formal submission should verify these sources directly before use. Third, the quantitative benchmarks compiled in Tables 2, 4, and 5 are drawn from studies that differ in testing protocol, scope, and independence of verification (ranging from an original primary claim, to independent expert critique, to direct observational monitoring data); readers should attend to the Source column in each table when weighing the strength of a given figure, rather than treating all reported values as equally well-established. Fourth, the pace of publication in AI-for-science research means that some very recent developments, particularly in generative materials modeling and operational space weather forecasting, may not be fully captured.

5. Conclusion

This review synthesized innovative AI-related research across materials discovery, nanostructured energy-storage engineering, and space weather physics, three domains that are individually well studied but rarely examined together, and grounded that synthesis in quantitative benchmarks drawn directly from the primary and critical literature (Tables 2–6). The evidence indicates a shared methodological pattern: in each domain, AI is used to navigate high-dimensional design or forecasting spaces that are intractable by classical forward methods alone — a 2.2-million-structure materials search space, an order-of-magnitude spread in electrode performance metrics, and multi-instrument solar-terrestrial observational data — and the most robust reported results combine AI with, rather than in place of, established physical theory.

At the same time, the quantitative record compiled here counsels caution alongside optimism. The GNoME case study demonstrates that even a landmark, highly cited AI-for-science result can substantially overstate its practically useful yield absent independent domain-expert verification (Cheetham & Seshadri, 2024); the wide spread of reported supercapacitor performance metrics underscores the need for standardized testing protocols before cross-study comparisons are drawn; and the substantial error in pre-cycle forecasts of Solar Cycle 25's amplitude — a smoothed peak of approximately 161 against a panel forecast of 115 — illustrates that even mature, multi-method forecasting approaches remain fallible at longer time horizons, a gap that motivates continued investment in AI-assisted forecasting without assuming it is already a solved problem. Realizing the full potential of this convergence will therefore require not only continued technical innovation but also deliberate investment in physics-informed model architectures, rigorous cross-domain benchmarking, independent critical appraisal as a routine part of the AI-for-science publication cycle, and interdisciplinary collaboration spanning computer science, chemistry, materials engineering, and heliophysics.

Future research should prioritize four directions in particular: (a) systematic, independently verified benchmarking of AI-generated materials candidates against experimentally validated ground truth, to establish realistic expectations for inverse-design pipelines and to avoid repeating the evaluation gap illustrated by the GNoME case; (b) standardized testing protocols for nanostructured electrode performance reporting, enabling meaningful cross-study comparison and integration of data-driven optimization directly into electrode design workflows; (c) extended-lead-time, physics-informed space weather forecasting models validated across a broader and more diverse set of historical solar-terrestrial events than the small number of extensively studied superstorms currently used as primary benchmarks; and (d) routine incorporation of independent, domain-expert critical appraisal into the AI-for-science publication and citation pipeline itself, given the demonstrated tendency for headline AI claims to accumulate citations well before rigorous independent scrutiny is applied.

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References

[1] Abdou Ahmed Abdou Elsehsah, K., Ahmad Noorden, Z., Mat Saman, N., et al. (2025). Graphene aerogel for supercapacitors: Influence of hydrothermal reduction parameters on electrochemical performance. Scientific Reports, 15, Article 41430. https://doi.org/10.1038/s41598-025-25844-1

[2] Agarwal, R., Mishra, R. K., & Mishra, D. (2026). Recent solar events and high-energy cosmic ray particles [Manuscript]. ResearchGate.

[3] Cheetham, A. K., & Seshadri, R. (2024). Artificial intelligence driving materials discovery? Perspective on the article: Scaling deep learning for materials discovery. Chemistry of Materials, 36(8), 3490–3495. https://doi.org/10.1021/acs.chemmater.4c00643

[4] Chemical & Engineering News. (2025, December). Duplicate structures haunt crystallography databases. American Chemical Society. https://cen.acs.org/research-integrity/Duplicate-structures-haunt-crystallography-databases/103/web/2025/12

[5] Cheng, M., Fu, C.-L., Okabe, R., et al. (2026). Artificial intelligence-driven approaches for materials design and discovery. Nature Materials, 25, 174–190. https://doi.org/10.1038/s41563-025-02403-7

[6] Guastavino, S., Legnaro, E., Massone, A. M., & Piana, M. (2025). Artificial intelligence could have predicted all space weather events associated with the May 2024 superstorm (arXiv:2501.14684). arXiv. https://arxiv.org/abs/2501.14684

[7] Merchant, A., Batzner, S., Schoenholz, S. S., Aykol, M., Cheon, G., & Cubuk, E. D. (2023). Scaling deep learning for materials discovery. Nature, 624(7990), 80–85. https://doi.org/10.1038/s41586-023-06735-9

[8] Mishra, R.K., Mishra, Divyansh and Agarwal, R. (2024), An Artificial Intelligence-Powered Approach to Material Design, In: Cutting-Edge Research in Chemical and Material Science Volume I, First Edition: August 2024, ISBN: 978-93-95847-39-1.

[9] Mishra, R.K., Mishra, Divyansh, and Agarwal, R. (2025), The future of materials science: Convergence of chemistry, physics, and artificial intelligence, In book: Materials Science Frontiers: From Chemical Principles to Physical Applications, October 2025, ISBN: 978-81-994425-3-5, 62-90..

[10] Mishra, Rajesh Kumar, Mishra, Divyansh and Agarwal, R. (2025). Design and optimization of nanostructured graphene–metal oxide composite electrodes for high-energy and long-cycle super capacitors, Journal of Science Research International (JSRI), ISSN: 2456 – 6365, DOI: 10.5281/zenodo.17442434, 11, 8, 22-35.

[11] Mishra, R.K., Mishra, Divyansh, and Agarwal, R. (2025), AI and Machine Learning in Physical Sciences, In: Frontiers of Physics: Multidisciplinary Research and Applications, An International Edition, Volume I, ISBN: 978-93-49938-05-2, 1-28.

[12] Mishra, Rajesh Kumar, Mishra, Divyansh and Agarwal, R. (2026). Artificial Intelligence in Space Weather Prediction: Advances, Benchmarks, and Future Directions, International Journal of Science, Architecture, Technology, and Environment, ISSN 3048-8222, Volume 03, Issue 03, March 2026, 823-842.

[13] Mishra, Rajesh Kumar, Mishra, Divyansh and Agarwal, R. (2026). Solar Cycle 25: The Largest in Two Decades Ground-Level Enhancements, Forbush Decreases, and the Evolving Space Weather Landscape, International Journal of Advanced Scientific and Technical Research, ISSN 2249-9954, Volume16, Issue. 2, 2026, 4/1-4/22.

[14] Mishra, R. K., Mishra, D., & Agarwal, R. (2026c). Real-time space weather prediction and geomagnetic storm forecasting, International Journal of Science, Engineering and Technology, 14, 3, 1-11.

[15] Mishra, R.K., Mishra, Divyansh, and Agarwal, R. (2026), Artificial intelligence for materials discovery and engineering, In book: Intelligent Computing and AI Frontiers: First Edition, Febtuary 2026, ISBN: 978-93-47587-80-1, 146-162.

[16] NOAA Space Weather Prediction Center. (2023). NOAA forecasts quicker, stronger peak of solar activity. National Oceanic and Atmospheric Administration. https://www.spaceweather.gov/news/noaa-forecasts-quicker-stronger-peak-solar-activity

[17] Solar Influences Data Analysis Center. (2024). Solar Cycle 25 reached its maximum in October 2024. Royal Observatory of Belgium. https://www.sidc.be/article/solar-cycle-25-reached-its-maximum-october-2024

[18] Yallur, B. C., Rao, M. P., Harshitha, M., Basrur, D., Umesh, P. H., Kamat, V., Venu Prasad, K. D., Venugopala, K. N., & Bhat, R. S. (2025). Recent advances in graphene-based metal oxide composites for supercapacitors: A comprehensive review. Advanced Sustainable Systems, 9(8), Article 2500121. https://doi.org/10.1002/adsu.202500121