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Editorial

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AI for Science: Paradigm shift or phase transition?

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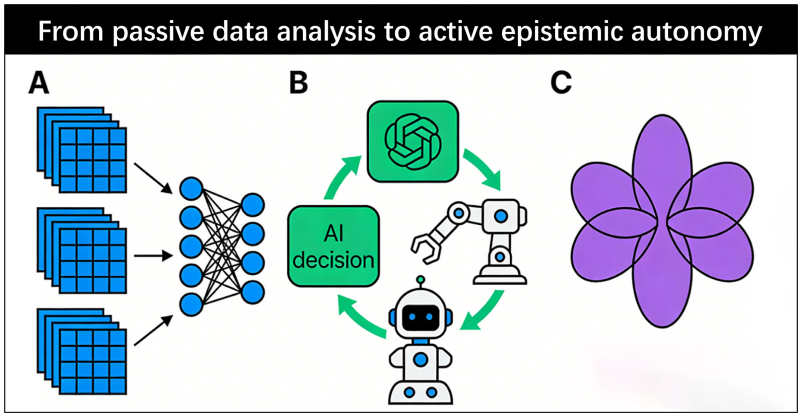
The 2024 Nobel Prizes in Physics and Chemistry have cemented artificial intelligence (AI) as a transformative force in scientific research, marking the mainstream emergence of AI for Science (AI4S). This editorial interrogates the core epistemological question facing the research community: whether AI-driven inquiry constitutes a fundamental paradigm shift in the scientific method or merely a transitional phase in computational data processing. We delineate the evolutionary tiers of AI capability in scientific discovery, namely, Keplerian, Edisonian, and Einsteinian AI, and analyze the pivotal shift toward agentic scientific systems that are redefining human-AI research collaboration. We further address the critical infrastructure gaps, ethical risks, and reproducibility challenges inherent to the mainstream adoption of AI4S, particularly within the environmental science disciplines. To uphold editorial rigor and scholarly integrity, we propose a framework for evaluating AI-enabled research contributions, emphasizing human oversight, transparent methodology, and responsible innovation. This editorial calls for rigorous, cross-disciplinary scholarship that harnesses AI's potential while safeguarding the core principles of scientific inquiry, positioning AI4S as a sustainable driver of discovery rather than a fleeting technological trend.

Keywords: AI for Science, Agentic Science, Ethical governance

Graphical abstract



A watershed moment for AI in scientific discovery

The 2024 Nobel Prizes in Physics and Chemistry stand as a defining milestone for artificial intelligence in scholarly research, recognizing both foundational advances in neural network design and breakthrough applications of AI that solved the 50-year grand challenge of protein structure prediction[1]. This moment formalizes the maturation of "AI for Science" (AI4S) as a legitimate, high-impact domain of scientific inquiry, yet it compels the research community to confront a critical epistemological divide: Is this wave of AI-driven research a genuine paradigm shift in the scientific method, or merely a

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phase transition in computational data handling? Beyond technological fanfare, this turning point demands deliberate reflection on how AI is reshaping research workflows, knowledge production, and the delicate boundary between human and machine contributions to scientific progress.

An evolutionary taxonomy of AI in scientific discovery

Recent scholarship has established a structured framework to categorize AI's evolving role in scientific discovery, outlining three successive generations of capability: Keplerian, Edisonian, and Einsteinian AI[2,3]. This taxonomy is not a mere descriptive exercise, but a critical lens for assessing methodological novelty, epistemic agency, and scholarly merit—standards that directly guide editorial evaluation for journals bridging computational science and environmental research.

Keplerian AI, named for Johannes Kepler's pattern-focused analysis of planetary observations, refers to machine learning systems that extract statistical regularities from static, pre-existing datasets. These tools excel at data mining, classification, and trend identification, accelerating descriptive analytics but operating strictly within established theoretical frameworks, with no capacity for iterative experimentation or causal inference[3]. As advanced pattern detectors, they represent incremental improvements to traditional research pipelines, expanding human computational capacity without redefining core scientific practices.

Edisonian AI marks a qualitative break from passive data analysis, embodying a closed-loop model of autonomous experimentation and iterative discovery rooted in the trial-and-error innovation ethos of Thomas Edison. These systems move beyond analytical tooling to design, run, and refine empirical experiments with limited human supervision, integrating hypothesis generation, laboratory execution, real-time data interpretation, and adaptive optimization into a unified workflow[2]. A landmark example is the autonomous robotic chemist that conducted hundreds of unsupervised trials to identify novel catalytic materials, demonstrating AI's ability to drive empirical discovery at scales and speeds beyond human reach alone. This generation of AI signals a shift from passive tool to active collaborator, closing the gap between observational analysis and physical intervention to produce actionable, empirically validated knowledge—an evolution that blurs the line between computational support and scientific agency.

Einsteinian AI remains the aspirational frontier of AI4S, defined by systems capable of foundational theoretical innovation: generating novel scientific laws, unifying conceptual frameworks, and developing paradigm-redefining hypotheses that transcend the limitations of training data and existing disciplinary boundaries. Unlike the incremental gains of Keplerian AI or the empirical autonomy of Edisonian AI, Einsteinian AI aims to reconfigure core scientific understanding, a feat requiring abstract reasoning, causal inference, and cross-disciplinary knowledge synthesis[4]. While targeted progress in theoretical modeling and hypothesis generation shows early promise, genuine paradigm-building AI remains unrealized, leaving open critical questions about the limits of current machine learning architectures and the future of human-AI co-creation in science.

The rise of Agentic Science: Redefining the human-AI partnership

The most consequential shift in modern AI4S is the move from assistive tooling to agentic systems—a transition labeled "Agentic Science" that is redefining the dynamics of human-AI research collaboration[2]. Powered by large language models, multimodal sensing platforms, and integrated laboratory automation, these agentic systems perform tasks once considered uniquely human: formulating testable hypotheses, designing rigorous experiments, interpreting complex datasets, and revising research strategies in real time[5]. This shift raises profound, unresolved epistemological challenges: how to assign scientific credit when AI initiates transformative hypotheses, how to preserve reproducibility when model reasoning is locked within opaque neural weights, and how to maintain scientific rigor as decision-making moves beyond human interpretability. These questions are far from abstract for environmental science, where AI is already deployed in climate modeling, biodiversity monitoring, and sustainable materials development—fields defined by large spatiotemporal scales, inherent uncertainty, and high-stakes real-world applications. As agentic systems become more widespread, the research community must establish clear guardrails to balance automation with academic accountability.

Infrastructure, integrity, and ethical governance for AI4S

Realizing the responsible potential of AI4S requires far more than algorithmic innovation; it demands robust, standardized infrastructure for data curation, model validation, and performance benchmarking. Initiatives such as the SciHorizon platform, developed by the Chinese Academy of Sciences Computer Network Information Center (2025)[6], address this gap by establishing systematic metrics for scientific dataset quality and cross-disciplinary AI model evaluation, laying the metrological foundation needed for credible AI4S research. Even so, infrastructure alone cannot guarantee scientific integrity, as highlighted by leading scholarly publishing standards[7]. AI may streamline administrative workflows, assist in peer reviewer matching, or flag potential research misconduct, but editorial discernment, ethical judgment, and scientific accountability remain inherently human responsibilities. This principle extends to research design: AI can generate candidate solutions and automate experiments, but human oversight is indispensable to validate novelty, interpret mechanistic insights, and prevent flawed inference.

The integration of AI into scientific practice carries measurable epistemic and ethical risks that require proactive governance and critical scrutiny. First, bias amplification poses a persistent threat: models trained on historical publication data may perpetuate disciplinary inequities, favor entrenched research paradigms, and marginalize innovative or underrepresented perspectives[8]. Second, algorithmic opacity erodes transparency, as black-box systems used in manuscript triage, peer review, or data analysis obscure decision pathways and undermine trust in scholarly processes. Third, the lack of mature standardized AI benchmarks jeopardizes reproducibility, with disparate models often producing divergent outputs from identical inputs, compromising the foundational scientific principle of replicability[4]. Ethically, these risks mandate strict transparency norms: Journals must disclose AI use in editorial processes, authors must declare AI assistance in manuscript preparation, and reviewers must be informed of AI involvement in research design to ensure informed consent and equitable scholarly participation.

A framework for evaluating AI-enabled scholarship

To support consistent evaluation of AI4S scholarship, we propose a pragmatic, non-hierarchical framework aligned with the evolutionary

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stages of AI capability. This framework clarifies contribution type and appropriate review metrics for authors, reviewers, and editorial boards, categorizing AI's role as Instrument, Assistant, Collaborator, or Agent with tailored assessment criteria: Instrumental AI is judged on predictive accuracy and computational robustness; assistive AI on reliability and workflow efficiency; collaborative AI on experimental novelty and interpretability; and agentic AI on the validity of autonomous discovery and real-world scientific impact. This framework avoids value judgments across AI generations, focusing instead on methodological rigor and scientific merit to maintain editorial consistency. By adopting this framework, *Artificial Intelligence & Environment* aims to streamline peer review, reduce ambiguity in AI-related submissions, and uphold high standards for publishable AI4S research.

Concluding remarks

As AI4S continues to evolve, the line between research method and methodological foundation will continue to blur, challenging centuries-old norms of scientific authorship, discovery, and understanding. For *Artificial Intelligence & Environment*, this evolution is not a distant theoretical concept but a present reality, with AI already reshaping how we model planetary change, monitor ecological systems, and develop sustainable solutions. We invite submissions that advance both AI applications in environmental science and critical scholarship on the epistemological, ethical, and practical shifts transforming our field. The era of AI-driven science is firmly upon us, but its trajectory—whether a fleeting phase transition or a lasting paradigm shift—will ultimately be shaped by the rigor, responsibility, and vision of the research community. Prioritizing transparency, reproducibility, and human-centric governance will be essential to ensuring that AI4S delivers enduring scientific value rather than short-term technological hype.

Author contributions

The authors confirm their contributions to the paper as follows: Guang-Guo Ying: Writing – original draft. Chang-Er Chen: Writing – review & editing. Pei Hua: Writing – review & editing. Jing-Yu Lin: Writing – review & editing. All authors reviewed the results and approved the final version of the manuscript.

Data availability

Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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Competing interests

The authors declare that they have no conflict of interest.

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