
AI for Science Needs Scientific Alignment

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Abstract

This position paper argues that realizing AI’s potential for science while protecting science as a knowledge-producing institution requires alignment to science’s epistemic goals and values—a challenge that neither general AI alignment nor responsible AI frameworks adequately address. As investment in AI for science grows, troubling patterns multiply: conflicting claims about fundamental capabilities, documented contraction of research toward AI-amenable problems, and benchmark-driven development disconnected from scientific needs. We contend that science is an inherently valuable epistemic system oriented toward human understanding—not merely prediction—and that its value and reliability depend on social infrastructure that is now threatened by misaligned AI integration. We propose a new field of study, scientific alignment: ensuring AI systems optimize for epistemic norms like traceability, self-consistency, and support for human comprehension (technical alignment), while developing governance structures that sustain science’s social infrastructure (systemic alignment). We outline concrete research directions and argue that the goal is not to constrain AI, but to ensure it serves the genuine aims of scientific inquiry.

1. Framing and Motivation

The rapid growth in AI for science brings shifts in how the scientific community understands AI’s role and the broader values of science. We observe troubling patterns that threaten to erode both the epistemological foundations of science and the critical role that science plays in human society. Empirical analysis reveals that AI adoption con-

tracts the focus of scientific fields, steering communities toward problems where AI shows measurable advances while neglecting others (Hao et al., 2026). The institutions that sustain science are already straining: peer review struggles to identify AI-generated content that introduces fabricated citations into the scientific record (GPTZero, 2026), while some principal investigators consider replacing trainees with AI systems—eroding the mentorship through which scientific judgment develops. Meanwhile, provocative claims circulate that scientific research will be obsolete within years,¹ reflecting confusion about what science is and aims to achieve.

These developments raise critical questions about what AI systems for science should be optimizing for and what structures should govern their integration into scientific practice. In this paper, we focus on *fundamental science*—research oriented toward understanding phenomena rather than prediction or application alone. This scope is deliberate: the epistemic goals that define this kind of science create distinct alignment requirements.

Science has proven uniquely effective at advancing humanity’s understanding of the natural world. Philosophical accounts of scientific progress emphasize that this success is fundamentally epistemic: science progresses by accumulating knowledge, approaching truth, or deepening our grasp of how nature works (Niiniluoto, 2025). Crucially, this epistemic achievement depends not only on technical progress but also on social processes. As (Strevens, 2020) argues, science’s power derives not from individual brilliance but from institutional structures—particularly the requirement that disputes be settled by empirical evidence—that reliably produce knowledge even from flawed and biased participants. These processes are now under threat by AI systems optimized for targets misaligned with scientific goals: predictive accuracy without understanding, benchmark performance that fails to generalize, or speed rather than insight. To preserve science as a dependable, self-correcting knowledge-producing institution and realize AI’s genuine potential within it, **we argue that AI for science needs scientific alignment: the scientific community needs ways**

¹See, e.g., panel discussion at the 2025 NeurIPS Machine Learning and the Physical Sciences Workshop.

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to surface shared epistemic goals and ensure, through technical and social structures, that AI systems support and advance them. We borrow the term “alignment” deliberately but distinguish our use from discourse around superintelligence or existential risk. Our concern is not speculative future scenarios but the ongoing erosion of scientific epistemology by systems optimizing the wrong targets.

Specifically, we call for investment in a new interdisciplinary research direction, *scientific alignment*. As further described in Sections 3 and 4, this encompasses both technical alignment (how AI systems design and optimization can be aligned to the specific goals and values of science) and systemic alignment (how social structures and institutions should govern AI in science). Importantly, scientific alignment applies broadly to different types of AI systems: from narrow, domain-specific models like AlphaFold to partially or fully agentic systems, as well as to AI embedded in the social infrastructure of science such as peer review, research papers production, education or literature synthesis. While low-level technical implementations will necessarily vary across these contexts, the overarching goals and the need to coordinated research investment are universal.

Evidence of the need for scientific alignment is substantial. Claims of “accelerating science” proliferate without meaningful engagement of what the aims of science are or what acceleration would mean (Bubeck et al., 2025). AI capability evaluation studies produce directly conflicting results: CORE-Bench Hard reports that AI systems can reproduce scientific research (Siegel et al., 2024), while astronomy-grounded ReplicationBench finds poor performance on the same scientific task (Ye et al., 2025). High profile results like DeepMind’s discovery of 2.2 million new crystals (Merchant et al., 2023) fail basic scientific criteria for novelty and utility (Cheetham & Seshadri, 2024). The social infrastructure of science is struggling to adapt: peer review systems built around human-written papers now face AI-generated text that changes the very criteria reviewers use to assess quality (Kusumegi et al., 2025). The integration of AI into scientific training risks degrading the development of critical skills needed to evaluate, interpret, and extend AI-generated results (Lee et al., 2025). These are not isolated failures but symptoms of a systematic misalignment between what AI systems are optimized for and what science requires.

Furthermore, these critical questions are largely neglected by current research agendas. General AI alignment focuses on broad behavioral properties and values like helpfulness, harmlessness, and honesty, aimed at making systems safe and useful across contexts (Askell et al., 2021; Bai et al., 2022a). Systematic critiques have documented fundamental limitations of this approach: it produces sycophantic behavior prioritizing agreeableness over accuracy, and faces the ‘value specification problem’—human values cannot be

fully captured in loss functions or preference data (Casper et al., 2023; Dahlgren Lindström et al., 2025). Crucially, alignment is context-dependent: a general system meant for use across diverse contexts is “unlikely to be able to distinguish [helpful from harmful cases] reliably, given their diversity, regardless of the amount of RLHF fine-tuning it undergoes” (Dahlgren Lindström et al., 2025). This means being helpful and harmless in general does not guarantee producing good science; domain-specific epistemic norms require domain-specific alignment.

Meanwhile, responsible AI guidelines for science focus on how scientists should use AI tools: (Resnik & Hosseini, 2025; Commission, 2024; Acquaviva et al., 2024). These are valuable but address a different question. RAI tells scientists how to use AI responsibly; alignment asks what AI systems should be built to optimize for and what institutional structures should govern them. The scientific community is beginning to recognize these gaps. While individual scientists have called for consideration of the risks of AI scientific agents (Tang et al., 2025), the impact of indiscriminate adoption (Trotta, 2025), the insidious role of hype in research with AI (Thais, 2024), and the need for improved protocols (Narayanan & Kapoor, 2025), there is no coordinated effort to study and develop the necessary technical and social infrastructure to ensure scientific alignment. Without significant and coordinated investment, we risk identifying problems without developing solutions.

Neglecting scientific alignment carries significant risks. As similar foundation models and benchmarks propagate across fields, methodological diversity erodes and resources flow toward computationally expensive but epistemically inappropriate tools. Diminishing returns to additional compute suggest that deploying general-purpose LLMs where bespoke models would suffice wastes resources and scientific opportunity (Hooker, 2025; Shukla, 2025). These consequences compound over time: scientific processes offloaded to AI systems erode the training through which scientific judgment develops (Trotta, 2025). At the extreme, the misguided belief that AI systems can fully automate science threatens the institutional foundations of science itself. If scientific understanding is conflated with prediction, and prediction with automated computation optimized for efficiency, the rationale for funding human inquiry collapses. Addressing these risks requires coordinated effort: scientific alignment.

2. Elucidating the Values of Science

To align a system requires a bearing, a direction by which to correct its own orientation. Scientific alignment is no exception, requiring a set of shared values as input to normatively construct the epistemology of science. Without an understanding of what scientists consider successes for scientific discovery, it remains impossible to gauge either the potential

value or danger posed by AI systems to the scientific community. It is not the aim of this paper to impose a universal taxonomy of shared values that fully underscores the epistemology of science as a knowledge-producing institution. Rather, we offer an initial attempt to articulate high-level goals that can serve as a starting point for the conversations urgently needed within the scientific community.

2.1. Science As Knowledge Production

Despite different goals and activities, diverse fields in science share a unifying aim: scientific understanding (De Regt, 2017; Krenn et al., 2022; Potochnik, 2017; Friedman, 1974). Understanding differs from other epistemic aims such as accurate prediction, explanation, or scientific knowledge. First and foremost, understanding is a cognitive achievement by epistemic *agents*. Understanding is not achieved by a print out of results; it requires an agent to take these results and engage with them in a way that enables grasping the mechanisms and dependencies linking phenomena together. Understanding involves answering why-questions and what-if-things-had-been-different questions, and applying knowledge to related yet different scenarios (Hills, 2016; Wilkenfeld, 2013).

Consider AlphaFold, a model which provides valuable knowledge about predicting protein folding and helps generate new possible proteins (Jumper et al., 2021). However, as a standalone prediction tool, AlphaFold falls short of the ultimate aim of understanding because it does not illuminate why proteins fold as they do or reveal the underlying mechanisms. Scientist Ellen Zhong puts the point succinctly: “right now, you just have this black box that can somehow tell you the folded states, but not actually how you get there” (Saplakoglu, 2024). AlphaFold’s achievement thus demonstrates that there is more science still to be done: the work of achieving genuine understanding. Scientific alignment, can help ensure AI contributes to that deeper goal.

Furthermore, the limits of prediction for achieving scientific understanding mean that having an oracle that produces correct predictions, often taken to be the moon-shot of AI driven science, would not actually be doing science. Accurate prediction alone does not guarantee that the predictions are tracking the actual mechanisms or causal dependencies that give rise to a phenomenon.

Moreover, science is inherently value laden in several respects. Whether we prioritize the reduction of false positives versus false negatives of a scientific theory or model depends on our background values, available resources, and interests (Douglas, 2000; Biddle, 2022; Johnson, 2023; Sullivan, 2022b). Scientific understanding also is value laden in that the particular (causal) dependencies that are relevant and constitute scientific understanding can change given our values and interests (Sullivan, 2025). The human interests and

values that go into juggling value tradeoffs of scientific theories and models are codetermined by deliberation among scientists and public stakeholders. Scientific oracles and prediction machines are ill-suited toward scientific deliberation because such decisions by their nature are collectively decided through criticism, debate, and alignment. Finally, good science raises new questions, not just answers existing ones—a capacity prediction machines lack.

2.2. Science As Social Epistemology

The production of scientific knowledge and understanding does not happen on its own, it requires participatory agents. Similarly, the framework under which science is evaluated, the process that determines what counts as reliable knowledge, is dependent on social structures. Science’s reliability as a knowledge-producing institution depends on social processes including peer review and criticism, replication, transmission, and the social accountability of scientists (Longino, 2020; Kitcher, 1993).

For example, peer review remains the primary mechanism for evaluating the veracity of a scientific result. This is not because peer review is infallible, but because it systematizes the scrutiny that scientific claims require. Knowledge replication and transmission also depend on social infrastructure: citation networks, journal prestige, and community uptake, although not perfect, all function as signals that help scientists allocate attention and trust. Finally, research ethics and scientific integrity require adjudication through social judgment—determining what constitutes misconduct, what counts as adequate disclosure, and how to weigh competing values are fundamentally collective enterprises.

These social processes are not incidental to science, they are constitutive of it—what makes science trustworthy as a knowledge-producing institution, distinguishing it from other forms of inquiry. This is not to claim that these systems function perfectly; the replicability crisis, biases in peer review, and failures of accountability are well documented (Baker, 2016; Heesen & Bright, 2021). Misaligned AI systems are exacerbating these cracks: LLMs hallucinate citations that do not exist, fabricate quotations, confidently present false claims as established findings, and introduce biases in citation selection (Athaluri et al., 2023; Linardon et al., 2025). Crucially, AI systems do not face accountability the way human scientists do: a scientist who fabricates data risks reputation, career, and social standing; an AI system risks none of these. This asymmetry means that preserving science’s social infrastructure also requires alignment, in particular, what we call systemic alignment (see Section 3.2: governance structures that maintain accountability, critical evaluation, and collective knowledge building as AI’s integration in science evolves.

3. Scientific Alignment

To make scientific alignment more concrete as a research field, we propose two complementary components. Both require the scientific community to surface shared epistemic goals and values—a process that is itself valuable (see Section 2). *Technical alignment* translates these goals into model interventions, ensuring that AI systems optimize for the right targets, while *systemic alignment* addresses the broader structures, processes, and norms that should govern AI within the scientific community. These components are interdependent: technical alignment without systemic alignment risks building well-designed tools that erode scientific institutions; systemic alignment without technical alignment leaves us with governance frameworks but no principled basis for what the governed systems should actually do.

3.1. Technical Alignment

Technical alignment requires identifying shared epistemic norms that should guide the design, training, and evaluation of AI systems for science. Without explicit attention to what science values, AI systems optimize for available proxies. Goodhart’s Law applies as forcefully here as in any other domain: when a measure becomes a target, it ceases to be a good measure (Manheim & Garrabrant, 2018). We already see this dynamic at work. Materials discovery systems like GNoME optimize for prediction of theoretically stable crystal structures while producing outputs that materials scientists describe as largely unsynthesizable and lacking utility (Cheetham & Seshadri, 2024). Agentic systems now explicitly optimize for conference acceptance as a proxy for scientific value (Lu et al., 2024)—yet publication metrics like h-index or acceptance rates are social byproducts of science, not measures of genuine understanding or discovery. To avoid such outcomes, AI systems for science should be evaluated against epistemic norms that reflect what makes scientific knowledge valuable; we identify several such norms below. Our proposed norms draw on established philosophy of science (Kuhn, 1977; McMullin, 2013; Keas, 2018).

Traceability: Science requires not just answers but justifications, chains of inference connecting claims to evidence and prior knowledge. Traceability is essential for criticism, replication, and transmission of knowledge (Fidler & Wilcox, 2026). AI systems that produce correct predictions through opaque processes fail this criterion, even when accurate.

Coherence: Scientific knowledge forms a coherent world model; new findings must cohere with established understanding or explicitly identify tensions (Šešelja & Straßer, 2014). AI systems for science should be internally consistent and produce outputs coherent with existing scientific knowledge, flagging rather than ignoring contradictions.

Verifiability: The outputs of an AI system should be check-

able against nature and prior knowledge (Sullivan, 2022a). AI systems should facilitate verification by producing outputs amenable to empirical scrutiny and comparison with established results.

Calibration: AI systems should support accurate uncertainty quantification, including appropriate propagation through multi-model pipelines. In science, uncertainty determines what conclusions can legitimately be drawn—a measurement with large error bars cannot support strong claims, and extrapolation is only warranted when uncertainties are well-characterized (Yu et al., 2022).

Intelligibility: As discussed in Section 2.1, the ultimate aim of scientific AI is understanding, not just prediction. AI systems should produce outputs that scientists can interrogate and reason with; explanations of what factors drive results, how changes in inputs would alter outputs, and where the boundaries of applicability lie.

These epistemic norms provide the philosophical foundation for technical scientific alignment. Making alignment targets explicit enables research directions (Section 4), like process reward mechanisms that support coherence and verifiability, interpretability techniques that help surface scientific reasoning, and improved evaluation artifacts that ensure construct validity within the system of science. Recent empirical work confirms this: for scientific agents, alignment between tools and task requirements matters more than the sophistication of reasoning frameworks (Alampara et al., 2025). This component of scientific alignment complements existing work in AI alignment while addressing domain-specific needs that general alignment cannot guarantee.

3.2. Systemic Alignment

Systemic alignment concerns the social structures, incentives, and governance of AI for science. Uncritical adoption of AI loses sight of the large systemic impact beyond the narrow confines of the individual adopter or their research group—effects that at scale risk undermining the very structures enabling scientific research. Yet the scientific community lacks dedicated forums for these debates; the risk is then that the use of AI in science follows an unreflected path of least resistance, importing practices from commercial AI development without adjustment for science’s distinct epistemic goals. Current reward systems—career progression, hiring, peer review, credit, funding—were not designed for this regime. Systemic alignment calls for participatory deliberation where scientists co-create guidelines aligned with the values outlined in Section 2. We provide several examples of critical questions such deliberation must address.

How does science verify results and update collective understanding? The reproducibility crisis predates AI, but AI-generated outputs compound the challenge while straining

the systems meant to address it. Peer review and community acceptance of new knowledge are increasingly overwhelmed; domain experts struggle to maintain meaningful overview of developments in their own fields, and judging the quality of work produced by opaque AI systems requires scrutiny that current review processes are not designed to provide (Ball, 2023). Scalable evaluation cannot mean abandoning human judgment. Systemic alignment encourages the scientific community to grapple with how to treat results produced by AI models. Are they open to criticism in the same way claims from human scientists are? Science depends on a skeptical stance toward new claims; overconfidence in AI outputs undermines the self-correcting capacity on which reliability depends.

What norms should govern dissemination, credit, and responsibility? These questions are already urgent. Analysis of NeurIPS 2025 found over 100 hallucinated citations across 51 accepted papers—fabricated references that survived peer review at the field’s premier venue (GPTZero, 2026). Models trained on AI-generated text exhibit progressive degradation (Shumailov et al., 2024), threatening the knowledge base on which future research depends. Agentic systems raise unresolved questions about credit and accountability that norms designed for human authors cannot answer. Systemic alignment demands the scientific community develop new frameworks for these challenges rather than inheriting defaults from other domains.

How do we preserve how science renews itself? Science regenerates across generations: established knowledge is passed on, wrong ideas are weeded out, and novel approaches extend the envelope of speculative knowledge. This process rests on mentorship and apprenticeship, through which emerging scientists learn from interaction with supervisors and experienced peers—acquiring tacit knowledge not found in any textbook (Polanyi, 1966). If funding bodies defund training opportunities in favor of agentic AI, this transmission will crumble, leaving no one capable of identifying when AI systems fail. Equally concerning is the homogenization of research directions toward AI-amenable problems (Hao et al., 2026). Curiosity-driven science, arising from genuine human interest, has historically produced unexpected breakthroughs; AI systems lack the capacity for such curiosity. Systemic alignment questions the often-undisputed stance that automating knowledge production will lead to good outcomes for science.

3.3. Methodological Pluralism

Science is not monolithic: different fields employ different methods, standards of evidence, and criteria for success. These differences reflect distinct epistemic challenges posed by different domains of scientific inquiry. Any framework for scientific alignment must also allow for such variation.

The epistemic norms we identify in Section 3 are universal across science, but their operational definitions may vary by field. Consider verifiability: in experimental sciences like particle physics or chemistry, verifiability typically means reproducibility—another laboratory or experiment should be able to perform the same experiment and obtain consistent results. In observational sciences like astronomy or climate science, phenomena cannot be rerun; verifiability instead means convergence of independent lines of evidence—multiple probes pointing to the same conclusion. But both are instantiations of the same epistemic norm, and thus, both benefit from the shared framework of scientific alignment.

Systemic alignment must similarly respect methodological pluralism. The institutional structures that support good science—peer review, credit attribution, training pipelines, publication norms—vary substantially across fields. Physics has embraced preprints and large collaborative authorships; biology maintains stricter norms around authorship order. These differences reflect distinct social epistemologies that have evolved to meet each field’s challenges. Governance frameworks for AI in science cannot assume a one-size-fits-all approach—field-specific norms will shape what appropriate AI integration looks like. Yet the challenges are structurally similar: every discipline must grapple with maintaining training pipelines, preserving critical evaluation, and preventing homogenization. A shared framework enables fields to learn from each other rather than reinventing solutions in isolation, while a common vocabulary rooted in scientific epistemology allows coordination that generic AI governance cannot. Moreover, the meta-goal of advancing human understanding unites these varied implementations, making scientific alignment a coherent research program with both shared technical foundations and domain-specific applications, like the field of science itself (Massimi, 2022).

4. Research Directions and Call to Action

This paper is a call to action. The challenges we have outlined—ensuring AI systems optimize for genuine scientific understanding while preserving the social infrastructure that makes science trustworthy—will not be met without deliberate, coordinated effort across the scientific and AI communities, as well as the funders and institutions that support them. Below we outline concrete research directions that can advance scientific alignment across both its technical and systemic dimensions.

Scientific Constitutional AI Constitutional AI offers a natural starting point for scientific alignment. This approach trains models to evaluate and revise their outputs according to explicit principles, making alignment values auditable rather than implicit in preference data (Bai et al., 2022b). This explicitness is particularly valuable for science, where epistemic norms are already largely articulated in philosoph-

ical and methodological literature—unlike general human preferences, which resist clean specification. Current AI systems used in science are shaped by task-specific performance metrics or inappropriate proxies like conference acceptance, neither of which capture the epistemic norms scientists actually need. A scientific constitution would encode norms like traceability, coherence, verifiability, calibration, and intelligibility, with principles such as “conclusions should be traceable to evidence and reasoning,” or “claims should be consistent with established findings or explicitly flag disagreements”. This approach parallels recent work on legal alignment, which derives constitutional principles from legal epistemology and professional norms (Kolt et al., 2026). Developing scientific constitutions requires collaboration between AI researchers and philosophers of science (Longino, 2020; Kitcher, 1993), and raises open technical questions: how to handle conflicts between principles, how to operationalize abstract norms for specific domains, and how to evaluate whether a constitution actually improves scientific reasoning rather than surface compliance.

Process Reward Models Process reward models offer a technical approach well-suited to scientific alignment. Unlike outcome-based reward models that evaluate only final answers, PRMs provide feedback on intermediate reasoning steps, rewarding how conclusions are reached, not just whether they are correct (Lightman et al., 2023). This distinction is crucial for science, where the process of inquiry is constitutive of the result’s epistemic status. A correct prediction derived from flawed reasoning or spurious correlations does not constitute scientific knowledge; traceability and verifiability require that the path to a conclusion be sound, not merely that the conclusion match observations.

General-purpose PRMs developed for mathematics or coding evaluate logical validity and correctness, but scientific reasoning involves additional dimensions: appropriate handling of uncertainty, connection to prior knowledge, acknowledgment of assumptions and limitations, and the distinction between correlation and causal explanation. Scientific PRMs would need to encode these domain-specific norms while sharing technical infrastructure with broader PRM research—methods for step-level supervision, process-outcome decomposition, and avoiding reward hacking. Collecting step-level supervision for scientific reasoning poses distinct challenges: unlike mathematics or coding, where correctness can often be automatically verified, scientific reasoning requires evaluating appropriate uncertainty handling, valid causal inference, and coherence with domain knowledge. Open questions include how to leverage domain simulators for automated feedback, how to structure expert annotation efficiently, and whether existing artifacts like peer review comments could provide training signal.

Interpretability for Scientific Reasoning Interpretability

research offers tools for verifying whether AI systems operate in ways scientists would endorse—but scientific interpretability differs from general interpretability in its goals and success criteria. General interpretability asks if we can understand what a model is doing; scientific interpretability asks if what the model is doing aligns with scientific principles and domain knowledge. The goal is not merely to explain model behavior to users, but to verify that AI systems—whether prediction models, simulation surrogates, or agentic systems—operate in accordance with the epistemic norms that allow their outputs to function as scientific knowledge. This makes interpretability for science a scientific alignment problem, not just an explainability problem.

Current interpretability methods fall short of what science requires. Feature saliency maps and attention visualizations may indicate which inputs influenced a prediction, but they rarely connect to the domain concepts that constitute scientific understanding. Scientific interpretability requires representations that map onto physical quantities, causal mechanisms, and theoretical constructs. Recent work suggests this is achievable: (Fear et al., 2025) demonstrate that physics foundation models develop internal representations corresponding to human-understandable physical concepts and that these representations can be manipulated to steer model behavior, inducing or removing specific physical features from simulations. This research direction also encompasses methods for embedding domain knowledge into model architectures, and, crucially, assessing when and how such knowledge actually improves scientific utility. Initial evidence indicates that theoretical benefits do not always materialize in practice, and careful empirical evaluation is needed to understand the conditions under which embedding scientific structure helps (Thais & Murnane, 2023).

Aligned Artifacts Once the values of science are understood, it then becomes important to craft artifacts that can gauge how well the values are being followed. As science is an epistemic system that demands measurability, these artifacts must provide a quantifiable manner to track the success of scientific alignment efforts. The artifacts themselves must also reflect what scientists value: traceability, coherence, verifiability, calibration, and intelligibility. One such type of artifact is benchmarks. While contemporary benchmarks hold some value as relative measurements of model performance, scientific benchmarks such as Frontier-Science (Wang et al., 2025) and MedQA (Jin et al., 2020) do not actualize the full desires of their target audience: the scientific community (Alaa et al., 2025). Such benchmarks suffer from construct validity issues as their target of evaluation is not representative of its analogous real-world task (Eriksson et al., 2025; Bean et al., 2025; Reuel et al., 2024). These validity issues stem from benchmark development occurring in a space with limited to no value elucidation. Without investments being made into studying the align-

ment of scientific benchmarks, we risk further misalignment when popular benchmarks bias future ones (Ott et al., 2022).

Another artifact type that can ensure evaluation validity for scientific alignment is experimental datasets. These datasets are no longer theoretical representations of real-world problems as with benchmarks, but are realistic scenarios that scientists work on in their own research. The construction of experimental datasets allows the evaluation of AI systems to be expanded to a plethora of task types that become more aligned with real, trustworthy scientific research (Authors, 2026). In domains where experimental data is expensive, curated experimental datasets enable more realistic models and AI-augmented workflows (Bhimji et al., 2025). Scientific alignment should not only be about steering AI systems development, but also advocating for the continual evolution of the epistemology of science.

HCI for Science Human-computer interaction research is essential for translating scientific alignment principles into tools scientists actually use. Even well-aligned AI systems can fail to serve scientific goals if the interface obscures their limitations, discourages critical engagement, or makes human oversight impractical. This is an alignment concern: tools that undermine scientist judgment or make verification difficult work against the epistemic norms we have outlined, regardless of the underlying model’s properties.

This applies to the full range of AI tools scientists use. Consider citation management: a tool surfacing every possibly related paper might seem maximally helpful, but it undermines the scientific norm that citations represent literature actually read and verified. A scientifically aligned citation tool would instead help scientists engage meaningfully with relevant work—surfacing disagreement, flagging retracted or contested findings, and supporting the kind of critical literature engagement that grounds scientific claims. Similar questions arise for AI writing assistants, coding copilots, and data analysis tools: are they designed to support scientific reasoning, or merely to increase throughput?

For agentic systems, the questions become more acute. The Agents4Science conference, the first venue where AI served as both authors and reviewers, found that the highest-quality submissions involved meaningful human collaboration—the best results came not from fully autonomous AI but from effective human-AI teaming (Bianchi et al., 2025). This finding underscores that the research question is not whether to include humans, but how to structure interaction to maximize scientific value. What forms of explanation support scientific judgment? When should AI systems defer to scientists? And how do we evaluate whether a tool supports or undermines the epistemic norms of a field?

Sociotechnical Systems Design Beyond tools and models, scientific alignment requires research on the sociotechni-

cal systems through which science operates. Peer review, conferences, publication norms, and credit attribution are not merely administrative infrastructure, they are the mechanisms through which science achieves its epistemic goals of verification, criticism, and collective knowledge-building.

Importantly, many of these research questions do not require AI at all. The question of what good peer review looks like—whether it actually provides the epistemic benefits claimed for it, and at what cost—is a standing question in philosophy of science that AI merely makes more urgent (Heesen & Bright, 2021). Scientific alignment provides a framework for asking what these systems actually optimize for and whether those targets align with epistemic goals. How might we redesign these systems, with or without AI, to better serve scientific understanding? Where AI does enter these systems, participatory design becomes essential (Friedman & Hendry, 2019). Scientists, not just AI developers, must shape how AI-assisted peer review, automated literature synthesis, or algorithmic credit attribution actually work, ensuring these systems continue to serve the epistemic and social functions that make science trustworthy.

Community Investment Finally, realizing these research directions requires investment in the scientific community itself. The challenges of scientific alignment cannot be addressed by AI researchers alone, nor by individual scientists adapting tools built for other purposes. We need dedicated spaces—workshops, cross-disciplinary collaborations, working groups—where scientists, AI researchers, and philosophers can articulate field-specific values and shape the systems that will govern their work. Some communities have begun this process. A recent collaboration across physics and philosophy of science called for the physics community to develop its own large-scale AI models according to the epistemic standards of the field, rather than ceding this work to commercial developers with different priorities (Barman et al., 2025). This is the kind of initiative scientific alignment demands: scientists taking active responsibility for how AI is integrated into their disciplines.

Such efforts require institutional support: funding agencies, universities, and professional societies must recognize that preserving science as a knowledge-producing institution requires deliberate investment—funding interdisciplinary research, creating professional incentives for engagement, and building infrastructure for ongoing dialogue. The alternative—ceding AI integration to priorities set elsewhere—risks not just the erosion of scientific epistemology, but the end of science as a human enterprise altogether.

5. Alternative Views

We consider several alternative views that might challenge the need for scientific alignment. The first holds that once

AI systems become sufficiently capable, human involvement in science becomes unnecessary—that fully autonomous AI scientists represent the natural and desirable endpoint of AI for science. We set aside speculative scenarios involving conscious or superintelligent AI whose understanding might genuinely substitute for humans; we see no scientific evidence that such systems are imminent, and these narratives risk distracting from the ongoing erosion of scientific epistemology that demands attention now. Under this view, scientific alignment would serve as distraction from the goal of fully automating science. However, this view conflates two distinct epistemic enterprises and misunderstands what science is and why it is valuable. As we have argued, science is not merely a prediction-generating system but a collective epistemic institution oriented toward human understanding, constituted by social processes of criticism, replication, and accountability. An oracle that produces correct answers without traceable reasoning, without connection to existing knowledge, and without supporting human comprehension is not doing science, it is providing a fundamentally different epistemic resource. We maintain that an oracle does not *replace* science, any more than a calculator replaces mathematics or a search engine replaces scholarship. Moreover, eliminating human scientists is not merely an epistemic loss but a social one: it would dismantle the communities, careers, and training pipelines through which scientific judgment develops, leaving no one capable of identifying when AI systems fail or of asking the questions that AI would never think to pursue. If what we value is human understanding of the natural world—the ability to answer why-questions, to grasp how phenomena connect, to apply knowledge to novel situations—then AI systems must be aligned to support that aim, not substituted for it.

A second view holds that a more general AI alignment is sufficient. For example, the RICE principles put forward in (Ji et al., 2023) position Robustness, Interpretability, Controllability, and Ethicality as guiding concepts for AI design and governance. These principles would naturally apply to AI in science. Given that a more general push towards alignment would be more efficient, there shouldn't be any need for tailoring alignment to science in particular.

The counter is that general standards do not equate to standards for proper scientific methodology. Interpretability may be useful in both general AI governance and scientific practice, but that does not mean that the standards of clarity or even the meaning of the word 'explanation' are the same (Kasirzadeh, 2021). General ethical guidelines do not necessarily satisfy the values of scientific research, in particular, the need to contextualize results and update shared knowledge models with credible new information. These assessments require what Kuhn called "reasonable agreement": field-specific, sometimes measurement-specific consensus among experts about what constitutes a meaningful

finding versus an erroneous one (Bokulich & Bocchi, 2024). Without attention to these epistemic particulars, AI systems may produce outputs that satisfy general alignment criteria while failing to meet the methodological standards that make science trustworthy.

A third view suggests that one could simply develop bespoke tools for specific scientific tasks without needing any overarching framework. Rather than forcing a general AI tool to conform to scientific standards, avoid the need for scientific alignment altogether by engineering a narrow tool for the specific job. This argument presupposes what it seeks to avoid: we must still define evaluation standards for a narrow tool. Without a framework articulating scientific values like traceability, consistency with prior knowledge, and support for human understanding, there is no principled basis for assessment. Tool developers would need deep domain expertise to construct appropriate standards ad hoc for each application, duplicating effort across fields and risking inconsistent or inadequate criteria. The framework we propose provides precisely this: a shared set of standards against which any AI system, and its role in the process of science, can be evaluated. Moreover, a fragmented approach of disconnected narrow tools, each developed in isolation, risks missing opportunities for cumulative progress—both in AI capabilities and in our understanding of what makes AI genuinely useful for science. Scientific alignment is not an alternative to building good tools; it is what enables us to recognize good tools when we build them.

6. Conclusion

We have argued that realizing the potential of AI for science—and protecting science as a knowledge-producing institution—requires alignment to the epistemic goals and values of science. This challenge is distinct from general AI alignment and responsible AI frameworks, neither of which address domain-specific epistemic norms nor safeguard the social infrastructure on which science depends. Scientific alignment operates at two levels: technical alignment ensuring AI systems optimize for critical epistemic norms; and systemic alignment developing governance structures that preserve the social epistemology of science. This is both a technical research program and a social one, requiring collaboration across AI, domain sciences, and philosophy of science. But above all, this paper is an urgent call to action. The scientific community cannot afford to cede the future of science to AI developers and those who would declare science "solved." We must take ownership of defining what our fields value, what success looks like, and how AI is integrated into our practices. The goal is not to constrain AI, but to ensure it serves the genuine aims of scientific inquiry—and to ensure that science, as a human institution oriented toward understanding, continues to thrive.

References

- Acquaviva, V., Barnes, E. A., Gagne, D. J., McKinley, G. A., and Thais, S. Ethics in climate ai: From theory to practice. *PLOS Climate*, 3(8):e0000465, 2024.
- Alaa, A., Hartvigsen, T., Golchini, N., Dutta, S., Dean, F., Raji, I. D., and Zack, T. Medical large language model benchmarks should prioritize construct validity, 2025. URL <https://arxiv.org/abs/2503.10694>.
- Alampara, N., Ríos-García, M., Gupta, C., Mannan, S., Miret, S., Krishnan, N. M. A., and Jablonka, K. M. Task alignment outweighs framework choice in scientific LLM agents. In *AI for Accelerated Materials Design - NeurIPS 2025*, 2025. URL <https://openreview.net/forum?id=7cbwuA5k0T>.
- Askill, A., Bai, Y., Chen, A., Drain, D., Ganguli, D., Henighan, T., Jones, A., Joseph, N., Mann, B., DasSarma, N., et al. A general language assistant as a laboratory for alignment. *arXiv preprint arXiv:2112.00861*, 2021.
- Athaluri, S. A., Manthena, S. V., Kesapragada, V. K. M., Yarlagadda, V., Dave, T., and Duddumpudi, R. T. S. Exploring the boundaries of reality: investigating the phenomenon of artificial intelligence hallucination in scientific writing through chatgpt references. *Cureus*, 15(4), 2023.
- Authors, A. Position: Ai for science should be made provably scientifically safe. Concurrent Submission to ICML, 2026.
- Bai, Y., Jones, A., Ndousse, K., Askell, A., Chen, A., DasSarma, N., Drain, D., Fort, S., Ganguli, D., Henighan, T., et al. Training a helpful and harmless assistant with reinforcement learning from human feedback. *arXiv preprint arXiv:2204.05862*, 2022a.
- Bai, Y., Kadavath, S., Kundu, S., Askell, A., Kernion, J., Jones, A., Chen, A., Goldie, A., Mirhoseini, A., McKinnon, C., et al. Constitutional ai: Harmlessness from ai feedback. *arXiv preprint arXiv:2212.08073*, 2022b.
- Baker, M. 1,500 scientists lift the lid on reproducibility, 2016.
- Ball, P. Is ai leading to a reproducibility crisis in science? *Nature*, 624(7990):22–25, 2023.
- Barman, K. G., Caron, S., Sullivan, E., de Regt, H. W., de Austri, R. R., Boon, M., Färber, M., Fröse, S., Golling, T., Lopez, L. G., et al. Large physics models: towards a collaborative approach with large language models and foundation models. *The European Physical Journal C*, 85(9):1066, 2025.
- Bean, A. M., Kearns, R. O., Romanou, A., Hafner, F. S., Mayne, H., Batzner, J., Foroutan, N., Schmitz, C., Korgul, K., Batra, H., et al. Measuring what matters: Construct validity in large language model benchmarks. *arXiv preprint arXiv:2511.04703*, 2025.
- Bhimji, W., Chakkappai, R., Chang, P.-W., Chou, Y.-T., Diefenbacher, S., Dudley, J., Elsharkawy, I., Farrell, S., Ghosh, A., Giordano, C., Guyon, I., Harris, C., Hashizume, Y., Hsu, S.-C., Khoda, E. E., Krause, C., Li, A., Nachman, B., Rousseau, D., Schöfbeck, R., Shooshtari, M., Schwarz, D., Ullah, I., Wang, D., and Zhang, Y. FAIR universe higgsML uncertainty dataset and competition. In *The Thirty-ninth Annual Conference on Neural Information Processing Systems Datasets and Benchmarks Track*, 2025. URL <https://openreview.net/forum?id=F48NfH4NFE>.
- Bianchi, F., Queen, O., Thakkar, N., Sun, E., and Zou, J. Exploring the use of ai authors and reviewers at agents4science. *Nature Biotechnology*, pp. 1–4, 2025.
- Biddle, J. B. On predicting recidivism: epistemic risk, tradeoffs, and values in machine learning. *Canadian Journal of Philosophy*, 52(3):321–341, 2022.
- Bokulich, A. and Bocchi, F. Kuhn’s 2nd law of thermodynamics?: Measurement, data, and anomalies. In Wray, K. B. (ed.), *Kuhn’s The Structure of Scientific Revolutions at 60*. Cambridge University Press, 2024.
- Bubeck, S., Coester, C., Eldan, R., Gowers, T., Lee, Y. T., Lupsasca, A., Sawhney, M., Scherrer, R., Sellke, M., Spears, B. K., et al. Early science acceleration experiments with gpt-5. *arXiv preprint arXiv:2511.16072*, 2025.
- Casper, S., Davies, X., Shi, C., Gilbert, T. K., Scheurer, J., Rando, J., Freedman, R., Korbak, T., Lindner, D., Freire, P., et al. Open problems and fundamental limitations of reinforcement learning from human feedback. *arXiv preprint arXiv:2307.15217*, 2023.
- Cheetham, A. K. and Seshadri, R. Artificial intelligence driving materials discovery? perspective on the article: Scaling deep learning for materials discovery. *Chemistry of Materials*, 36(8):3490–3495, 2024.
- Commission, E. Living guidelines on the responsible use of generative ai in research., 2024.
- Dahlgren Lindström, A., Methnani, L., Krause, L., Ericson, P., de Rituerto de Troya, Í. M., Coelho Mollo, D., and Dobbe, R. Helpful, harmless, honest? sociotechnical limits of ai alignment and safety through reinforcement learning from human feedback: Ad lindström et al. *Ethics and Information Technology*, 27(2):28, 2025.

- De Regt, H. W. *Understanding scientific understanding*. Oxford university press, 2017.
- Douglas, H. Inductive risk and values in science. *Philosophy of science*, 67(4):559–579, 2000.
- Eriksson, M., Purificato, E., Noroozian, A., Vinagre, J., Chaslot, G., Gomez, E., and Fernandez-Llorca, D. Can we trust ai benchmarks? an interdisciplinary review of current issues in ai evaluation. *arXiv preprint arXiv:2502.06559*, 2025.
- Fear, R. A., Mukhopadhyay, P., McCabe, M., Bietti, A., and Cranmer, M. Physics steering: Causal control of cross-domain concepts in a physics foundation model. *arXiv preprint arXiv:2511.20798*, 2025.
- Fidler, F. and Wilcox, J. Reproducibility of Scientific Results. In Zalta, E. N. and Nodelman, U. (eds.), *The Stanford Encyclopedia of Philosophy*. Metaphysics Research Lab, Stanford University, Spring 2026 edition, 2026.
- Friedman, B. and Hendry, D. G. *Value Sensitive Design: Shaping Technology with Moral Imagination*. MIT Press, Cambridge, MA, 2019.
- Friedman, M. Explanation and scientific understanding. *the Journal of Philosophy*, 71(1):5–19, 1974.
- GPTZero. GPTZero finds 100 new hallucinations in NeurIPS 2025 accepted papers, 2026. URL <https://gptzero.me/news/neurips/>.
- Hao, Q., Xu, F., Li, Y., and Evans, J. Artificial intelligence tools expand scientists’ impact but contract science’s focus. *Nature*, pp. 1–7, 2026.
- Heesen, R. and Bright, L. K. Is peer review a good idea? *The British Journal for the Philosophy of Science*, 2021.
- Hills, A. Understanding why. *Noûs*, 50(4):661–688, 2016.
- Hooker, S. On the slow death of scaling. Available at SSRN 5877662, 2025.
- Ji, J., Qiu, T., Chen, B., Zhang, B., Lou, H., Wang, K., Duan, Y., He, Z., Zhou, J., Zhang, Z., et al. Ai alignment: A comprehensive survey. *arXiv preprint arXiv:2310.19852*, 2023.
- Jin, D., Pan, E., Oufattole, N., Weng, W.-H., Fang, H., and Szolovits, P. What disease does this patient have? a large-scale open domain question answering dataset from medical exams, 2020. URL <https://arxiv.org/abs/2009.13081>.
- Johnson, G. M. Are algorithms value-free?: Feminist theoretical virtues in machine learning. *Journal of Moral Philosophy*, 21(1-2):27–61, 2023.
- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., et al. Highly accurate protein structure prediction with alphafold. *nature*, 596(7873):583–589, 2021.
- Kasirzadeh, A. Reasons, values, stakeholders: A philosophical framework for explainable artificial intelligence. In *Proceedings of the 2021 ACM Conference on Fairness, Accountability, and Transparency*, pp. 14–14, 2021.
- Keas, M. N. Systematizing the theoretical virtues. *Synthese*, 195(6):2761–2793, 2018.
- Kitcher, P. *The advancement of science: Science without legend, objectivity without illusions*. Oxford University Press, 1993.
- Kolt, N., Caputo, N., Boeglin, J., O’Keefe, C., Bommasani, R., Casper, S., Cuéllar, M.-F., Feldman, N., Gabriel, I., Hadfield, G. K., et al. Legal alignment for safe and ethical ai. *arXiv preprint arXiv:2601.04175*, 2026.
- Krenn, M., Pollice, R., Guo, S. Y., Aldeghi, M., Cervera-Lierta, A., Friederich, P., dos Passos Gomes, G., Häse, F., Jinich, A., Nigam, A., et al. On scientific understanding with artificial intelligence. *Nature Reviews Physics*, 4(12):761–769, 2022.
- Kuhn, T. S. Objectivity, value judgment and theory choice. in: *The essential tension*. Urbana: University of Illinois Press, 1977.
- Kusumegi, K., Yang, X., Ginsparg, P., de Vaan, M., Stuart, T., and Yin, Y. Scientific production in the era of large language models. *Science*, 390(6779):1240–1243, 2025.
- Lee, H.-P., Sarkar, A., Tankelevitch, L., Drosos, I., Rintel, S., Banks, R., and Wilson, N. The impact of generative ai on critical thinking: Self-reported reductions in cognitive effort and confidence effects from a survey of knowledge workers. In *Proceedings of the 2025 CHI conference on human factors in computing systems*, pp. 1–22, 2025.
- Lightman, H., Kosaraju, V., Burda, Y., Edwards, H., Baker, B., Lee, T., Leike, J., Schulman, J., Sutskever, I., and Cobbe, K. Let’s verify step by step. In *The Twelfth International Conference on Learning Representations*, 2023.
- Linardon, J., Jarman, H. K., McClure, Z., Anderson, C., Liu, C., and Messer, M. Influence of topic familiarity and prompt specificity on citation fabrication in mental health research using large language models: experimental study. *JMIR Mental Health*, 12:e80371, 2025.
- Longino, H. E. Science as social knowledge: Values and objectivity in scientific inquiry. 2020.

- Lu, C., Lu, C., Lange, R. T., Foerster, J., Clune, J., and Ha, D. The ai scientist: Towards fully automated open-ended scientific discovery. *arXiv preprint arXiv:2408.06292*, 2024.
- Manheim, D. and Garrabrant, S. Categorizing variants of goodhart’s law. *arXiv preprint arXiv:1803.04585*, 2018.
- Massimi, M. *Perspectival realism*. Oxford University Press, 2022.
- McMullin, E. The virtues of a good theory. In *The Routledge companion to philosophy of science*, pp. 561–571. Routledge, 2013.
- Merchant, A., Batzner, S., Schoenholz, S. S., Aykol, M., Cheon, G., and Cubuk, E. D. Scaling deep learning for materials discovery. *Nature*, 624(7990):80–85, 2023.
- Narayanan, A. and Kapoor, S. Why an overreliance on ai-driven modelling is bad for science. *Nature*, 640(8058): 312–314, 2025.
- Niiniluoto, I. Scientific Progress. In Zalta, E. N. and Nodelman, U. (eds.), *The Stanford Encyclopedia of Philosophy*. Metaphysics Research Lab, Stanford University, Winter 2025 edition, 2025.
- Ott, S., Barbosa-Silva, A., Blagec, K., Brauner, J., and Samwald, M. Mapping global dynamics of benchmark creation and saturation in artificial intelligence. *Nature Communications*, 13(1), November 2022. ISSN 2041-1723. doi: 10.1038/s41467-022-34591-0. URL <http://dx.doi.org/10.1038/s41467-022-34591-0>.
- Polanyi, M. *The Tacit Dimension*. Doubleday, Garden City, NY, 1966.
- Potochnik, A. Idealization and the aims of science. In *Idealization and the Aims of Science*. University of Chicago Press, 2017.
- Resnik, D. B. and Hosseini, M. The ethics of using artificial intelligence in scientific research: new guidance needed for a new tool. *AI and Ethics*, 5(2):1499–1521, 2025.
- Reuel, A., Hardy, A., Smith, C., Lamparth, M., Hardy, M., and Kochenderfer, M. J. Betterbench: Assessing ai benchmarks, uncovering issues, and establishing best practices. *Advances in Neural Information Processing Systems*, 37:21763–21813, 2024.
- Saplakoglu, Y. How ai revolutionized protein science, but didn’t end it. *Quanta Magazine*. June, 26, 2024.
- Šešelja, D. and Straßer, C. Epistemic justification in the context of pursuit: A coherentist approach. *Synthese*, 191(13):3111–3141, 2014.
- Shukla, H. The ai scaling wall of diminishing returns: Of llms, electric dogs, and general relativity. *arXiv preprint arXiv:2512.20264*, 2025.
- Shumailov, I., Shumaylov, Z., Zhao, Y., Papernot, N., Anderson, R., and Gal, Y. Ai models collapse when trained on recursively generated data. *Nature*, 631(8022):755–759, 2024.
- Siegel, Z. S., Kapoor, S., Nagdir, N., Stroebel, B., and Narayanan, A. Core-bench: Fostering the credibility of published research through a computational reproducibility agent benchmark. *arXiv preprint arXiv:2409.11363*, 2024.
- Strevens, M. *The knowledge machine: How an unreasonable idea created modern science*. Penguin UK, 2020.
- Sullivan, E. Understanding from machine learning models. *British Journal for the Philosophy of Science*, 73(1):109–133, 2022a. doi: 10.1093/bjps/axz035.
- Sullivan, E. Inductive risk, understanding, and opaque machine learning models. *Philosophy of Science*, 89(5):1065–1074, 2022b.
- Sullivan, E. Value encroachment on scientific understanding and discovery. *Philosophical Studies*, pp. 1–21, 2025.
- Tang, X., Jin, Q., Zhu, K., Yuan, T., Zhang, Y., Zhou, W., Qu, M., Zhao, Y., Tang, J., Zhang, Z., et al. Risks of ai scientists: prioritizing safeguarding over autonomy. *Nature Communications*, 16(1):8317, 2025.
- Thais, S. Misrepresented technological solutions in imagined futures: The origins and dangers of ai hype in the research community. In *Proceedings of the AAAI/ACM Conference on AI, Ethics, and Society*, volume 7, pp. 1455–1465, 2024.
- Thais, S. and Murnane, D. Equivariance is not all you need: characterizing the utility of equivariant graph neural networks for particle physics tasks. *arXiv preprint arXiv:2311.03094*, 2023.
- Trotta, R. The indiscriminate adoption of ai threatens the foundations of academia. *Nature Astronomy*, pp. 1–2, 2025.
- Wang, M., Lin, R., Hu, K., Jiao, J., Chowdhury, N., Chang, E., and Patwardhan, T. Frontierscience: Evaluating ai’s ability to perform expert-level scientific tasks, 2025.
- Wilkenfeld, D. A. Understanding as representation manipulability. *Synthese*, 190(6):997–1016, 2013.
- Ye, C., Yuan, S., Cooray, S., Dillmann, S., Roque, I. L., Baron, D., Frank, P., Martin-Alvarez, S., Koblichke, N., Qu, F. J., et al. Replicationbench: Can ai agents

replicate astrophysics research papers? *arXiv preprint arXiv:2510.24591*, 2025.

Yu, J., Wang, D., and Zheng, M. Uncertainty quantification: Can we trust artificial intelligence in drug discovery? *Isience*, 25(8), 2022.