

AI4Research: A Survey of Artificial Intelligence for Scientific Research

Qiguang Chen^{1*} Mingda Yang^{1*} Libo Qin^{2,✉} Jinhao Liu¹ Zheng Yan¹ Jiannan Guan¹
 Dengyun Peng¹ Yiyuan Ji¹ Hanjing Li¹ Mengkang Hu³ Yimeng Zhang⁴ Yihao Liang⁵
 Yuhang Zhou⁶ Jiaqi Wang⁷ Zhi Chen⁸ Wanxiang Che^{1,✉}

¹ LARG, Research Center for Social Computing and Interactive Robotics, Harbin Institute of Technology,

² School of Computer Science and Engineering, Central South University, ³ The University of Hong Kong,

⁴ University of Illinois Urbana-Champaign, ⁵ Princeton University, ⁶ Fudan University,

⁷ Chinese University of Hong Kong, ⁸ ByteDance Seed (China)

Abstract:

Recent advancements in artificial intelligence (AI), particularly in large language models (LLMs) such as OpenAI-o1 and DeepSeek-R1, have demonstrated remarkable capabilities in complex domains such as logical reasoning and experimental coding. Motivated by these advancements, numerous studies have explored the application of AI in the innovation process, particularly in the context of scientific research. These AI technologies primarily aim to develop systems that can autonomously conduct research processes across a wide range of scientific disciplines. Despite these significant strides, a comprehensive survey on AI for Research (AI4Research) remains absent, which hampers our understanding and impedes further development in this field. To address this gap, we present a comprehensive survey and offer a unified perspective on AI4Research. Specifically, the main contributions of our work are as follows: (1) **Systematic taxonomy**: We first introduce a systematic taxonomy to classify five mainstream tasks in AI4Research. (2) **New frontiers**: Then, we identify key research gaps and highlight promising future directions, focusing on the rigor and scalability of automated experiments, as well as the societal impact. (3) **Abundant applications and resources**: Finally, we compile a wealth of resources, including relevant multidisciplinary applications, data corpora, and tools. We hope our work will provide the research community with quick access to these resources and stimulate innovative breakthroughs in AI4Research.

* Equal Contribution

✉ Corresponding Author

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 Projects: <https://ai-4-research.github.io>

 Code Repository: <https://github.com/LightChen233/Awesome-AI4Research>

 Contact: qgchen@ir.hit.edu.cn, car@ir.hit.edu.cn, lbqin@csu.edu.cn

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1. Introduction

In recent years, the rise of artificial intelligence (AI), particularly large language models (LLMs) like DeepSeek-R1 [265], has stimulated significant research in the field of reasoning. These breakthroughs have notably improved the models' performance across diverse areas, including mathematical reasoning, programming, and interdisciplinary knowledge [727, 751, 619, 941, 957, 111]. Some of these models have even surpassed the Turing Test [354], marking a pivotal achievement in AI development. Inspired by these, a series of works attempts to explore advanced AI systems for innovative tasks, especially in the scientific discovery of new research [869, 894, 853, 958]. Earlier, the AI Scientist [509] introduces the concept of a fully automatic AI for research system, which divides the research process into three key stages: idea mining, experiment conduction, and academic writing. Initially, the system generates and evaluates novel ideas and hypotheses. Once a hypothesis is formulated, experiments are conducted automatically, producing results that include numerical data and visual summaries. These results are presented in tables and images, followed by an interpretation with a convincing description, culminating in a LaTeX report. In the final stage, the AI Scientist generates an automated review that refines the project and provides feedback for future open scientific discoveries. Similarly, other classic models, such as Carl [332] and Zochi [12], follow broadly analogous workflows. Notably, AgentArxiv [668] and AgentLab [669] assign distinct roles to multiple agents to simulate the collaborative nature of scientific research teams, incorporating additional peer review, academic survey, enabling semi-automatic and even full-automatic collaboration rather than relying on a single agent [480, 876, 113, 661, 53]. More recently, Swanson et al. [735] extend LLMs' scientific reach by

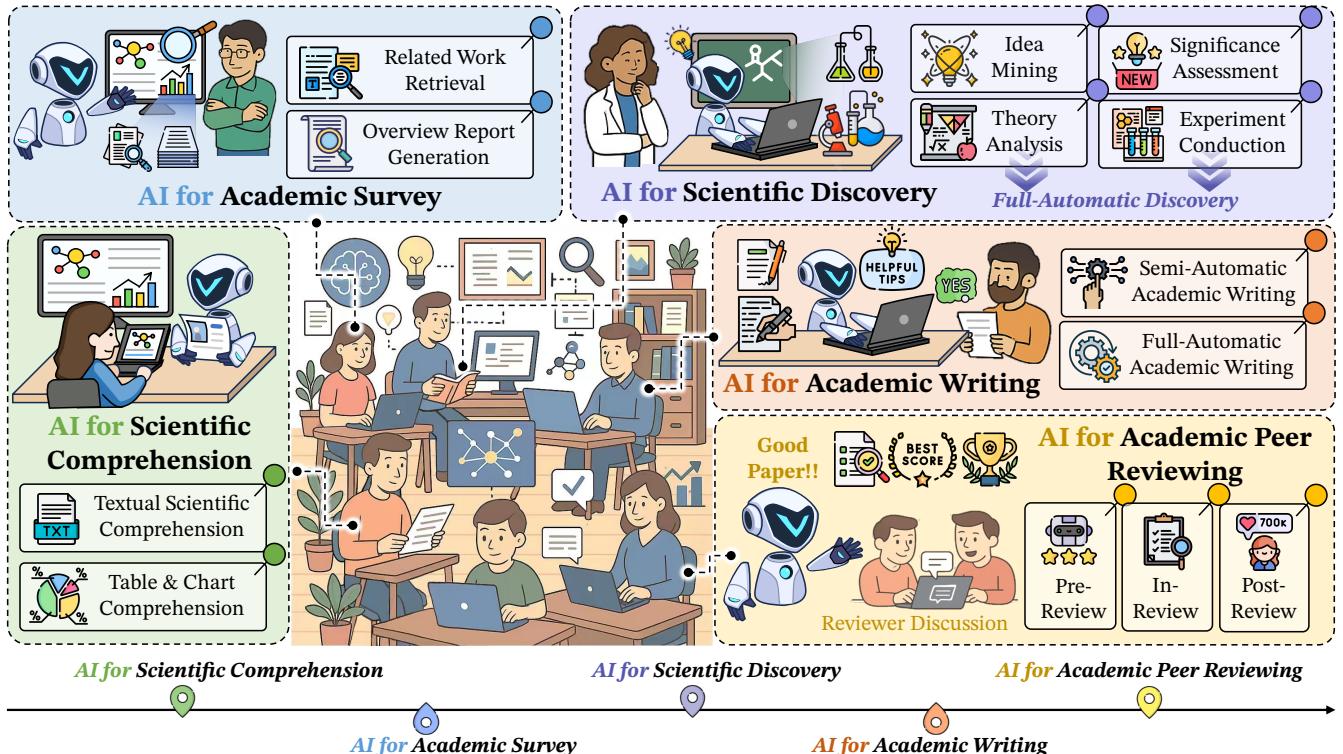


Figure 1: The mainstream processes and categories of AI4Research, which can be divided into five key areas: (1) AI for Scientific Comprehension, (2) AI for Academic Survey, (3) AI for Scientific Discovery, (4) AI for Academic Writing, and (5) AI for Academic Peer Review. Each of these areas contributes to improving the effectiveness and efficiency of AI-integrated research and publication.

presenting the Virtual Lab, an AI-human platform that designs nanobody binders for emerging SARS-CoV-2 variants, underscoring the promise of such collaboration for research. Despite these advancements, there remains a lack of comprehensive surveys to systematically analyze the key factors and recent developments in AI-driven research, which significantly impedes the continued progress of this field.

To address this gap, we first define and present a comprehensive survey of AI for research, termed AI4Research. As shown in Figure 1, we **introduce a systematic taxonomy of AI4Research**, focusing on the following areas: (1) *AI for Scientific Comprehension*: AI systems' ability to extract relevant information from scientific literature is crucial; (2) *AI for Academic Surveys*: This involves AI techniques for systematically reviewing and summarizing scientific literature; (3) *AI for Scientific Discovery*: AI is used to generate hypotheses, theories, or models based on existing scientific knowledge; (4) *AI for Academic Writing*: AI tools support researchers in drafting, editing, and formatting manuscripts; (5) *AI for Academic Reviewing*: AI assists in evaluating and providing feedback on scientific manuscripts. Given the vast literature, we **highlight promising future research in AI4Research**. Future work should prioritize interdisciplinary AI models that integrate knowledge across scientific domains to encourage cross-disciplinary collaboration. Addressing ethical concerns and biases within AI systems is crucial for ensuring fairness and transparency in research. Improving the explainability of AI models and exploring adaptive, real-time systems for dynamic scientific experiments will be vital for advancing AI's role in research. Additionally, we **suggest key applications and valuable resources in AI4Research**, such as representative multidisciplinary applications, open-source frameworks, and datasets repositories to support further studies. We introduce AI for Natural Science research, AI for Applied Science and Engineering research, and AI for Social Science research. Finally, we review tools essential for model development and public benchmarks that provide rich data for training and experimentation.

The main contributions of this work are as follows:

- **Systematic Taxonomy for AI in Research:** This paper introduces a comprehensive taxonomy of AI applications in research, spanning five areas: scientific comprehension, academic surveys, scientific discovery, academic writing, and academic reviewing. It categorizes AI tools that enhance and even automatically execute various stages of the research process.
- **Emerging Future Research Areas:** The paper identifies key future research avenues for AI in academia, including the development of interdisciplinary AI models, addressing ethical concerns and biases, improving model explainability, and exploring adaptive AI systems for dynamic scientific experiments.
- **Key Applications and Abundant Trending Resources:** We present multidisciplinary applications of AI4Research across natural sciences, applied science, and social sciences. It also identifies essential resources, open-source frameworks, public datasets, collaborative platforms, and academic tools, that facilitate discovery management and AI-driven research.

2. The Definition of AI4Research

AI4Research denotes the application of artificial intelligence methods to improve, accelerate, and partially automate research across disciplines. To clarify this paradigm, as shown in Figure 2, we identify six core capabilities: AI for Scientific Comprehension, AI for Academic Survey, AI for Scientific Discovery, AI for Academic Writing, AI for Academic Peer Reviewing. Each of them illustrates a distinct way that AI advances the research process. Formally, let $\mathcal{T} = \{T_{SC}, T_{AS}, T_{SD}, T_{AW}, T_{PR}\}$ be the set of research tasks, Scientific Comprehension, Academic Survey, Scientific Discovery, Academic Writing, and Peer Reviewing. For each task $T_i \in \mathcal{T}$, there exists a corresponding AI model A_i that is specifically tailored to address the requirements of

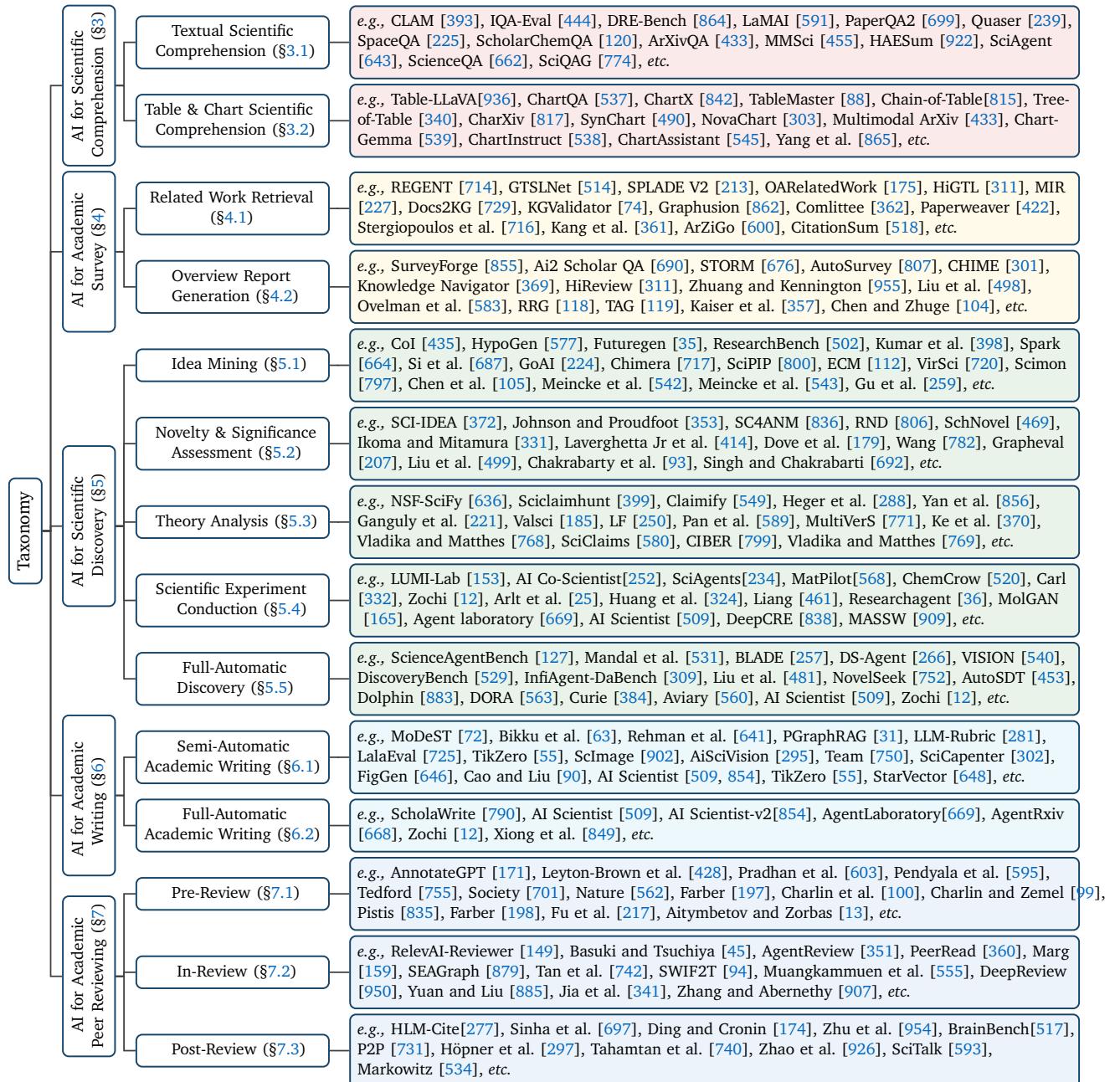


Figure 2: The taxonomy of AI for research (AI4Research) is categorized into five key areas. Each area is subdivided into specific tasks, underscoring the varied roles of AI in the entire research process.

that task. Then the overall AI4Research system can be expressed as the functional composition:

$$\mathcal{A} = A_{\text{PR}} \circ A_{\text{AW}} \circ A_{\text{SD}} \circ A_{\text{AS}} \circ A_{\text{SC}}, \quad (1)$$

where \circ denotes the function composition operator, meaning that the output of one function becomes the input of the next. Furhter, applied to a research query q (or more generally to an interactive research-query lifecycle \mathcal{Q}), we can obtain:

$$\mathcal{A}(q) = (A_{\text{PR}} \circ A_{\text{AW}} \circ A_{\text{SD}} \circ A_{\text{AS}} \circ A_{\text{SC}})(q). \quad (2)$$

The objective of an AI4Research system is to maximize research lifecycle efficiency, application performance, and innovation capacity, namely:

$$\max \{ \eta(\mathcal{A}(\mathcal{Q})), \alpha(\mathcal{A}(\mathcal{Q})), \tau(\mathcal{A}(\mathcal{Q})) \}, \quad (3)$$

where $\eta(\cdot)$, $\tau(\cdot)$, and $\alpha(\cdot)$ evaluates the efficiency, performance, and innovation of the generated research publications $\mathcal{A}(\mathcal{Q})$, respectively.

2.1. Component-wise Definition of AI4Research

We now define and formalize each core module in the AI4Research framework.

2.1.1. AI for Scientific Comprehension

AI for Scientific Comprehension (AI4SC) is central to AI4Research, enabling extraction, interpretation, and synthesis of information from a single scientific literature. This accelerates human knowledge acquisition and improves the efficiency of automated analysis. Formally, we define this module to gain knowledge K after comprehension as a composite reasoning function:

$$\hat{\mathcal{K}} = A_{SC}(\mathcal{K}) = f_{SC}(\mathcal{K}|D_{SC}, \Phi_{SC}) = f_{TCSC} \circ f_{TSC}(\mathcal{K}|D_{SC}, \Phi_{SC}), \quad (4)$$

where A_{SC} is the comprehension AI model to extract the possible knowledge \mathcal{K} ; the documents $D_{SC} = \{D_T, D_F, D_M\}$ comprises texts (D_T), figures (D_F), and other metadata (D_M); Φ_{SC} includes model parameters and domain priors; and f_{SC} means the specific comprehension algorithms, including a textual comprehension function f_{TSC} that extracts and interprets textual content, and a table & chart comprehension function f_{TCSC} that analyzes tables and charts.

The goal of AI4SC is to maximize scientific understanding σ with extracted knowledge $\hat{\mathcal{K}}$ from the original documents D_{SC} :

$$\max\{\sigma\} = \max\{\mathbb{E}_{\hat{\mathcal{K}} \sim A_{SC}}[\text{Coherence}(\hat{\mathcal{K}}, D_{SC}) + \text{Coverage}(\hat{\mathcal{K}}, D_{SC})]\}, \quad (5)$$

where Coherence measures logical consistency; Coverage quantifies concept completeness between them.

2.1.2. AI for Academic Survey

AI for Academic Survey (AI4AS) is designed to synthesize and structure multiple existing literature, providing a comprehensive overview of a research domain. This enhances the ability to identify trends, gaps, and key contributions in scientific fields. Formally, we define this module to generate a structured literature survey S as a functional synthesis function:

$$\hat{S} = A_{AS}(S) = f_{AS}(S|R_{AS}, \Phi_{AS}) = f_{Gen} \circ f_{Retrieval}(S|R_{AS}, \Phi_{AS}), \quad (6)$$

where A_{AS} is the survey AI model to generate the possible survey S ; R_{AS} comprising survey domain requirements; Φ_{AS} includes model parameters and domain priors; f_{AS} means the specific survey algorithms, which include a retrieval function $f_{Retrieval}$ that retrieves relevant literature based on the query, and a generative function f_{Gen} that produces thematic clusters and summaries.

The objective of AI4AS is to maximize survey quality ρ of the generated survey \hat{S} with respect to the requirement R_{AS} :

$$\max\{\rho\} = \max\{\mathbb{E}_{\hat{S} \sim A_{AS}}[\text{Relevance}(\hat{S}, R_{AS}) + \text{Coverage}(\hat{S}, R_{AS}) + \text{Clarity}(\hat{S}, R_{AS})]\}, \quad (7)$$

where Relevance measures the match between documents and the target topic; Coverage assesses the breadth and depth of the domain; Clarity reflects the coherence, abstraction quality, and utility of the synthesized representation based on the generated survey and requirements.

2.1.3. AI for Scientific Discovery

AI for Scientific Discovery (AI4SD) is focused on generating, and validating novel scientific hypotheses or ideas and conducting experiments or simulations. This module enhances the ability to explore uncharted scientific territories and accelerate innovation. Formally, we define this module to generate, validate, and implement scientific innovations $\hat{\mathcal{I}}$ as a discovery-oriented function:

$$\hat{\mathcal{I}} = A_{SD}(\mathcal{I}) = f_{SD}(\mathcal{I}|K_{SD}, R_{SD}, \Phi_{SD}) = f_{ED} \circ f_{TA} \circ f_{NSA} \circ f_{IM}(\mathcal{I}|K_{SD}, R_{SD}, \Phi_{SD}), \quad (8)$$

where A_{SD} is a discovery-oriented AI to explore possible innovation \mathcal{I} ; scientific knowledge $K_{SD} = \{K_D, K_{AS}\}$ is the given domain knowledge (K_D) and recent related-work summarized knowledge (K_{AS}) derived from upstream comprehension and survey stages; R_{SD} means the research requirement; Φ_{SD} includes model parameters and domain priors; f_{SD} means the specific discovery algorithms, which include a generative function f_{IM} that mines candidate ideas, a novelty and significance assessment function f_{NSA} that evaluates the quality and importance of each idea candidates, a theory analysis function f_{TA} that checks theoretical soundness, and an experiment conduction function f_{ED} that makes plans and executes experiments then finally complete the scientific discovery.

The goal of AI4SD is to maximize the total discovery quality δ of the generated innovations $\hat{\mathcal{I}}$:

$$\max\{\delta\} = \max\{\mathbb{E}_{\hat{\mathcal{I}} \sim A_{SD}} [\text{Novelty}(\hat{\mathcal{I}}) + \text{Validity}(\hat{\mathcal{I}}) + \text{Significance}(\hat{\mathcal{I}})]\}, \quad (9)$$

where Novelty evaluates innovativeness; Validity assesses experimental and theoretical soundness; Significance reflects the follow-up impact of the study.

2.1.4. AI for Academic Writing

AI for Academic Writing (AI4AW) is a highlight section of AI4Research, assisting researchers in generating, revising, and formatting scientific manuscripts. This module enhances the quality and efficiency of academic writing, ensuring that manuscripts are well-structured and compliant with publication standards. Formally, we define this module to generate a publication-ready manuscript \mathcal{M} as a collaborative writing function:

$$\hat{\mathcal{M}} = A_{AW}(\mathcal{M}) = f_{AW}(\mathcal{M}|K_{AS}, \text{Info}_I, \Phi_{AW}) = f_{DWP} \circ f_{DMW} \circ f_{AWC}(\mathcal{M}|K_{AS}, \text{Info}_I, \Phi_{AW}), \quad (10)$$

where A_{AW} denotes a writing-oriented AI to generate the possible manuscript \mathcal{M} ; Info_I is all information in the scientific discovery stage, including ideas, experimental designs, and attachments such as codes and data; Φ_{AW} includes model parameters and domain priors; f_{AW} means the specific writing algorithms, which include a during-manuscript-preparation function f_{DWP} that prepares the manuscript structure, a during-manuscript-writing function f_{DMW} that generates the manuscript content, and a after-manuscript-completion function f_{AWC} that completes grammatical corrections, expressions and logical modifications.

The objective of AI4AW is to maximize writing quality and effectiveness ω of the manuscript $\hat{\mathcal{M}}$:

$$\max\{\omega\} = \max\{\mathbb{E}_{\hat{\mathcal{M}} \sim A_{AW}} [\text{Consistency}(\hat{\mathcal{M}}) + \text{Readability}(\hat{\mathcal{M}}) + \text{Compliance}(\hat{\mathcal{M}})]\}, \quad (11)$$

where Consistency reflects logical flow and internal coherence; Readability measures linguistic clarity and ease of understanding; Compliance assesses adherence to formatting and stylistic requirements.

2.1.5. AI for Academic Peer Reviewing

AI for Academic Peer Reviewing (AI4PR) is a critical component of AI4Research, automating and enhancing the peer review process. This module aims to provide structured, objective, and constructive reviews of

	AI4Science	AI4Research
Scope	Scientific Discovery, Data Analysis.	Broader Research workflows.
Goal	Scientific Breakthroughs.	Publications, Methods, Overall Productivity.
Applications	Material Discovery, Drug Design, Genomics, etc.	Comprehension, Writing, Peer Review, etc.
Target Users	Research Experts.	Both Research Experts and New Scientists.

Table 1: Comparison and discussion between AI4Science and AI4Research, especially in terms of scope, goal, applications, and target users.

scientific manuscripts, improving the quality and efficiency of the review cycle. Formally, we define this module to generate a structured review result R as an evaluative reasoning function:

$$\hat{R} = A_{PR}(\mathcal{R}) = f_{PR}(\mathcal{R}|P, \Phi_{PR}) = f_{PostP} \circ f_{InP} \circ f_{PreP}(\mathcal{R}|\hat{\mathcal{M}}, \Phi_{PR}), \quad (12)$$

where A_{PR} denotes a review-oriented AI to generate the possible review \mathcal{R} ; Φ_{PR} includes model parameters and domain priors; f_{PR} means the specific review algorithms, which include a pre-review function f_{PreP} that completes pre-review preparations, an in-review function f_{InP} that generates or augments review reports, and a post-review function f_{PostP} that completes post-review analysis of papers.

The goal of AI4PR is to maximize review quality θ of the review result \hat{R} based on the manuscript $\hat{\mathcal{M}}$:

$$\max\{\theta\} = \max\{\mathbb{E}_{\hat{R} \sim A_{PR}}[\text{Correctness}(\hat{R}, \hat{\mathcal{M}}) + \text{Helpfulness}(\hat{R}, \hat{\mathcal{M}}) + \text{Consistency}(\hat{R}, \hat{\mathcal{M}})]\}, \quad (13)$$

where Correctness means the review can correctly reflect the pros and cons of research; Helpfulness measures the depth, constructiveness, and usefulness of feedback; Consistency quantifies the alignment of the review with established evaluation criteria and domain standards.

2.2. Discussion About AI4Science and AI4Research

Since the concepts of AI4Science and AI4Research share many similarities, as outlined in Table 1, it is important to distinguish the key differences between the two. **AI4Science (Artificial Intelligence for Science)** focuses on applying AI technologies to accelerate scientific discovery and data analysis across various fields, including material discovery, drug design, and genomic analysis. Its primary objective is to integrate AI into research workflows to support experts in achieving significant scientific advancements. In contrast, **AI4Research (Artificial Intelligence for Research)** adopts a broader perspective, addressing publications, methodologies, and overall research productivity. It emphasizes AI's role in enhancing research methods and supporting the academic environment for both established researchers and emerging scientists. Key applications in this domain include AI-driven tools for literature comprehension, academic writing assistance, and peer review processes.

The core distinction between these frameworks lies in their focus: AI4Science targets specific scientific problems and experimental protocols, while AI4Research addresses broader research methodologies and academic infrastructure. However, as LLMs develop more advanced reasoning and generative capabilities, a unified workflow is emerging that can address both specialized scientific challenges and general research processes. Consequently, AI4Science tools are increasingly integrated into AI4Research environments, often serving as callable components in LLM-based systems for scientific exploration. Subsequently, we will provide a detailed analysis of our taxonomy and the relevant literature.

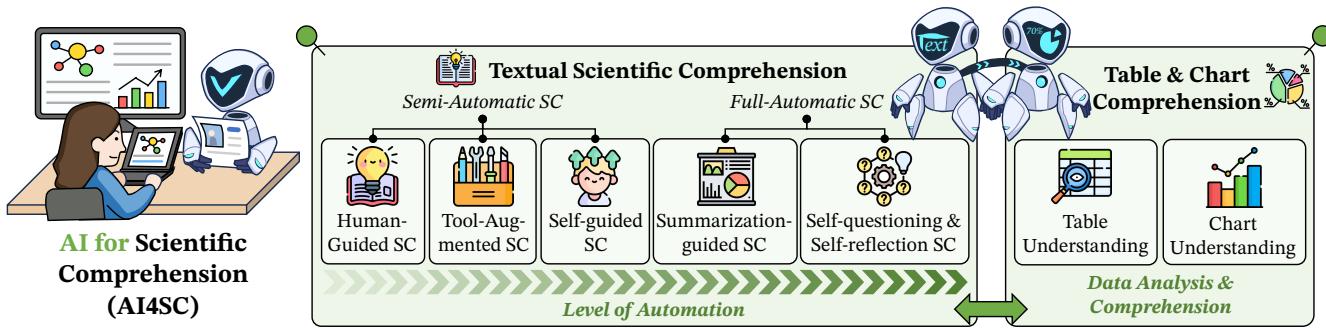


Figure 3: The primary paradigms of AI for Scientific Comprehension. These include: (1) Textual Scientific Comprehension, which is further categorized into Semi-Automatic and Fully-Automatic Scientific Comprehension; and (2) Table & Chart Scientific Comprehension, encompassing Table and Chart Understanding.

3. AI for Scientific Comprehension

Scientific comprehension plays a pivotal role in advancing AI4Research, encompassing the ability to extract, understand, and synthesize information from the scientific literature. This capability not only accelerates human understanding and knowledge acquisition but also enhances the efficiency of automatic analysis, enabling more effective research processing. As shown in Figure 3, it contains two main categories: Textual Scientific Comprehension (§ 3.1) and Table & Chart Scientific Comprehension (§ 3.2).

3.1. Textual Scientific Comprehension

Textual Scientific Comprehension refers to the ability to understand, interpret, and critically evaluate scientific texts. It involves identifying key concepts, grasping complex terminology, and synthesizing information to form a cohesive understanding of scientific principles and findings [624, 70, 533]. As depicted in Figure 3 (middle), we categorize the corresponding comprehension technologies into two types based on automation level: Semi-Automatic and Fully-Automatic Scientific Comprehension.

3.1.1. Semi-Automatic Scientific Comprehension

Semi-automatic scientific comprehension denotes systems in which, given a manually created question, the AI produces comprehensive question-related comprehension of long-context scientific content. Such systems support both researchers and AI models in deepening their grasp of complex scientific concepts [120, 292, 823]. Specifically, these systems comprise three main categories:

Human-Guided Scientific Comprehension is an interactive approach where researchers and language models engage in iterative dialogues to produce a deepened understanding of questions on complex scientific literature step-by-step [393, 903, 444, 864, 616]. LaMAI [591] equips language models with “active inquiry” capabilities: before providing a definitive answer, the model asks clarifying questions to resolve ambiguities in user queries, reducing misinterpretations and enhancing relevance [854]. These platforms illustrate that embedding structured human feedback loops within LLM-based tools improves output reliability and enriches the scientific discovery process by uncovering latent questions and assumptions. However, the approach requires significant human-AI interaction, which can increase costs.

Tool-Augmented Scientific Comprehension refers to cases where a researcher’s query surpasses a language model’s knowledge base or its context-window limit [827]. The model then invokes several external tools to ensure accurate output: (1) **Knowledge Retrieval Tool** uses retrieval-augmented generation to inject

knowledge beyond the model's training [380, 662]. Early systems like document-centric agents [407] extract key findings, note limitations, and propose future directions. Graphusion [862] advances this by building scientific knowledge graphs and extracting entity triples, resolving conflicts across disciplines without manual effort. SiGIR [137] uses self-critique feedback to guide the iterative reasoning process during knowledge-intensive multi-hop reasoning tasks. (2) **Fact Checking Tool** mitigates hallucinations and factual errors by applying verification modules to reduce the AI's hallucinations [356, 280, 251, 917]. PaperQA2 [699] integrates rigorous factuality checks and matches or exceeds expert accuracy on literature-review tasks, all without unrestricted Internet access or human oversight. (3) **Reasoning-Augmentation Tool** addresses limited logical reasoning and computation in standalone models to deepen the AI's theory-level comprehension [111]. For example, SciAgent [524] dynamically selects calculators and formula evaluators to deliver precise, domain-specific reasoning. Collectively, these advances show how coupling AI with specialized tools transforms scientific workflows from passive consumption into an interactive, tool-powered process that accelerates discovery while preserving rigor.

Self-guided Scientific Comprehension refers to a model's capacity to respond to a single-turn query regarding a scientific publication with a comprehensive, context-sensitive answer [56, 653, 71]. Earlier, Clark et al. [144] demonstrate that even seemingly factual questions about academic papers require deep contextual understanding and meticulous attention to document-specific details [239]. To address these challenges, subsequent studies focus more on enhanced semi-automatic scientific comprehension in long-context papers [489, 746], particularly in specialized fields such as aerospace science [225], chemistry [597, 120], and clinical medicine [639, 696]. It illustrates that enhancing models to align with the linguistic and conceptual conventions of each discipline, particularly those with improved long-context capabilities, leads to significant advancements [126, 500]. Furthermore, recognizing the inherently multimodal nature of scientific papers, several studies have begun to integrate textual analysis with figures and charts [433, 455, 643], thereby advancing towards a more holistic, paper-wide comprehension of scientific content.

3.1.2. Full-Automatic Scientific Comprehension

AI for full-automatic scientific comprehension refers to the ability of an AI system to read and understand scientific knowledge independently without human questions or other intervention. The goal of such systems is to fully automate the processing of scientific literature, the formulation and answering of complex questions, and even, to some extent, scientific discovery or idea mining.

Summarization-guided Automatic Scientific Comprehension refers to the capability of LLMs to autonomously generate summaries of scientific articles and, based on these summaries, construct a comprehensive narrative of the research [371, 212]. This process enhances the model's holistic understanding of lengthy scientific texts and mitigates comprehension biases that arise from processing extensive documents in a purely token-by-token manner [922]. Furthermore, Ifargan et al. [330] suggest that LLMs can further enhance their overall comprehension of lengthy scientific documents through the generation of autonomous summaries. Their approach utilizes a system of multiple agents, such as a Summary Agent and a Proofreading Agent, working collaboratively to extract and refine experimental results and research methodologies without human intervention. This ultimately produces a refined abstract suitable for peer review.

Self-Questioning & Self-Reflection Automatic Scientific Comprehension involve an AI generating and answering its own questions or reflection to deepen its understanding of scientific content [313, 550, 875]. Earlier, SciInstruct [896] proposes a self-reflective annotation framework, where a model generates step-by-step reasoning for unlabeled scientific questions and then refines its output through self-critique, producing high-quality annotations. Building on this, several studies [516] have focused on prompting models to autonomously create question sequences that enhance their comprehension of scientific texts. One notable

example is SciQAG [774], which proposes a pipeline where a “question generator” and an “answer evaluator” collaborate to extract diverse, research-level comprehension from scientific papers.

More recently, LLMs have been directed to self-improve by posing clarifying questions and decomposing complex problems in a Socratic style, strengthening reasoning and conceptual understanding [625, 708, 816]. The Introspective Growth [834] further refines this approach, prompting smaller models to generate fundamental, open-ended questions that guide larger models toward better task comprehension. This process integrates external text retrieval to refine the understanding of technical semantics.

3.2. Table & Chart Scientific Comprehension

Beyond pure textual content, LLMs are employing various techniques to more efficiently interpret and leverage information from tables and figures, thereby achieving a deeper and more comprehensive understanding of scientific literature [142, 564, 268].

3.2.1. Table Understanding

Table understanding involves methods that enable LLMs to extract, interpret, and infer data from tables in scientific literature [721, 837, 28]. **(1) Data Augmentation:** The most direct way is to add higher quality table understanding data. For instance, Zheng et al. [936] introduce the MMTab dataset for large-scale multimodal table understanding in a generative format and propose Table-LLaVA, which reasons directly on table images through instruction tuning, demonstrating the great advantage of visually grounded table representations. **(2) Reasoning Paradigm Augmentation:** Subsequent work explores suitable reasoning paradigms [88, 912, 777, 778]. Wang et al. [815] propose Chain-of-Table, which incrementally constructs and updates tables within an LLM’s reasoning chain to improve comprehension of complex tables. Ji et al. [340] introduce Tree-of-Table, hierarchically condensing and decomposing large tables into a tree structure to facilitate LLM reasoning. Cao and Liu [88] present TableMaster, a framework that enhances LLM table understanding by extracting and verbalizing relevant table content with enriched semantic context and adaptively switching between textual and symbolic reasoning.

3.2.2. Chart Understanding

Chart Understanding involves techniques enabling multimodal large language models to directly process and interpret chart images in scientific papers, supporting tasks such as question answering and summarization based on chart content [605, 465, 546, 321]. Furthermore, several studies focus on assembling and synthesizing large, diverse chart datasets to improve chart understanding [490, 303, 433]. Masry et al. [538] and Meng et al. [545] present vision-language instruction datasets for charts, and train both end-to-end and pipeline models that achieve state-of-the-art results on scientific chart understanding tasks [539]. Further, Yang et al. [865] propose the Formalized Description for Visualization (FDV), a structured textual representation of charts that enables large language models to learn for diverse and deeper comprehension.

4. AI for Academic Survey

It is widely acknowledged that a thorough and well-conducted pre-writing survey and research phase forms the cornerstone of a successful academic article [649]. Inspired by this, AI for Academic Survey is proposed to systematically review and summarize scientific literature through the application of artificial intelligence techniques. This process plays a crucial role in ensuring that researchers and automated systems remain current with the latest advancements in their field and can efficiently identify relevant studies to inform their own work. As shown in Figure 4, it contains two main stages: Related Work Retrieval (§ 4.1) and Overview Report Generation (§ 4.2).

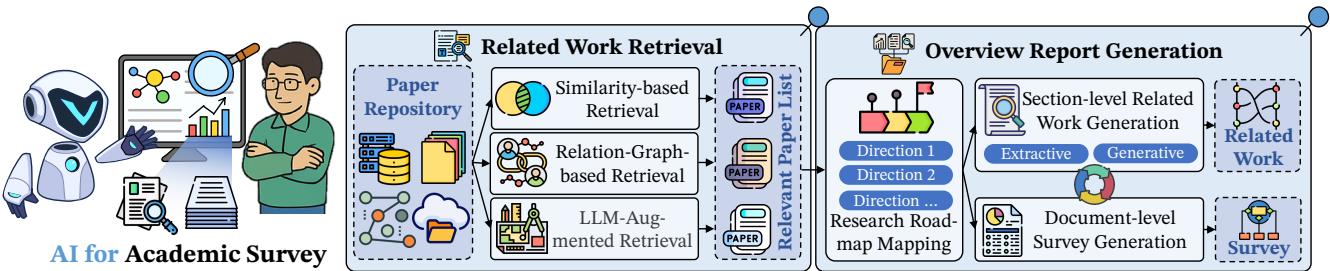


Figure 4: The two primary stages in AI-driven academic surveys: Related Work Retrieval and Overview Report Generation. Related Work Retrieval is further subdivided into Semantic-Guided Retrieval, Graph-Guided Retrieval, and LLM-Augmented Retrieval. Overview Report Generation encompasses Research Roadmap Mapping, Section-level Related Work Generation, and Document-level Survey Generation.

4.1. Related Work Retrieval

Related Work Retrieval entails AI proactively identifying foundational and novel research papers aligned with their evolving scientific objectives [52, 457, 674, 194]. Existing research divides into three paradigms:

Semantic-Guided Retrieval involves identifying relevant literature by matching the semantic representation extracted from a user query to the terms present in documents based on similarity [37, 388, 447]. In the biomedical domain, GTSLNet [514] enhances semantic-guided retrieval by utilizing a group-based keyword similarity learning network, which automatically selects clinically analogous studies. Similarly, SPLADE V2 [213] advances neural retrieval by integrating sparse lexical signals with dense expansion models, achieving significant results. Moreover, Garikaparthi et al. [227] concentrate on inspiration retrieval to provide enhanced support for idea mining.

Graph-Guided Retrieval models scholarly entities (e.g., papers, authors, citations) as a graph [74, 729, 862, 716]. Based on the types and granularity of nodes, this search method can be categorized into three types: (1) **Author Relationship Graph** captures the connections between researchers, enabling searches based on author relationships. For example, author-relationship graphs can effectively model collaboration networks and researcher influence [362, 600]. Building on this concept, Kang et al. [361] developed a “user-recommended paper” knowledge graph that traces users’ interactions with literature, enhancing recommendation transparency and trust. (2) **Paper Relationship Graph** is always constructed using citation relationships between papers to construct broader paper relationships [311]. CitationSum [518] creates a citation graph linking target papers to their references with weighted relevance scores, then uses graph contrastive learning to produce abstractive summaries. (3) **Entity Relationship Graph**: can be constructed by modeling relationships between logical entities within papers, enabling more precise retrieval. For example, Li and Ouyang [448] propose a graph-based model that automatically identifies inter-paper entity relationships, such as contrast and support, guiding the construction of a structured Related Work section. Cross-domain graph methods are increasingly used in interdisciplinary research. Further, to address complex questions such as “Which synthesis pathways enable material X to achieve optimal conductivity?”, Ye et al. [872] systematically extract entities and their relationships from the materials science literature, thus enhancing the depth of exploration.

LLM-Augmented Retrieval involves leveraging the capabilities of LLMs to improve search effectiveness and result quality by integrating them with academic retrieval systems. (1) **Single-Agent Retrieval**: The most straightforward approach is to employ a single AI model as a standalone agent to accomplish the retrieval task. For instance, Lee et al. [422] introduce the PaperWeaver framework, which places an LLM-based

agent atop a graph to enable deeper reasoning, thereby enhancing interpretability in classification and recommendation tasks. **(2) Multi-Agent Retrieval:** Beyond single-agent systems, several studies employ multiple specialized agents to simplify retrieval and increase accuracy [670, 498, 689]. LitLLMs [9] splits the automatic literature review into two subtasks: retrieval and generation. It proposes a two-phase LLM pipeline that extracts keywords from abstracts and reranks results to improve recall. Liu et al. [498] propose a multi-agent framework for full-text related-work generation, which includes a selector to choose sections to read, a reader to update shared memory, and a writer to generate the related work section. The framework uses graph-aware strategies to optimize the reading order of references. **(3) Deep Research:** Recent research has advanced this paradigm towards more autonomous “Deep Research” [578, 579], where AI agents perform the end-to-end research process, from exploration and synthesis to generating citation-rich reports [865, 181, 942]. This progress is enabled by novel agent architectures that emulate human research heuristics [829]. For instance, the PaSa agent [287] discovers literature by actively traversing citation networks. Concurrently, the retrieval strategies themselves have become more intelligent; the ExSearch framework [680] allows an agent to continuously optimize its search strategies through a self-incentivization loop, while CuriousLLM [868] employs a “curiosity-driven” mechanism where the agent actively generates questions to guide its retrieval process of knowledge graphs.

4.2. Overview Report Generation

Based on retrieved data, automated generation of structured, coherent overview reports has become essential in academic writing and AI4Research process [293]. According to the writing sequence, we need to first complete the research roadmap mapping, followed by the generation of section-level related work, and finally produce the complete document-level survey.

4.2.1. Research Roadmap Mapping

Research Roadmap Mapping refers to the process of cleaning, integrating, and depicting the developmental trajectories of a research topic by synthesizing insights from a broad corpus of literature [8, 855, 690, 807]. This methodology is crucial for enhancing the rigor and completeness of literature surveys and meta-analyses, as it enables researchers to discern emerging trends, unresolved gaps, and potential future directions more systematically [111, 69, 855]. Specifically, Zhu et al. [948] demonstrate that organizing a survey into a hierarchical structure significantly improves coherence [676].

Recently, more interactive hierarchical frameworks have also emerged. CHIME [301], for instance, refines LLM-generated structures through iterative human-AI collaboration. Similarly, Katz et al. [369] expand this to a two-tiered hierarchy, effectively organizing extensive surveys. Further, HiReview [311] illustrates the benefits of multilayered tree structures for systematic knowledge organization. Moreover, Zhuang and Kennington [955] propose a graph-based taxonomy that categorizes LLM survey papers into defined classes, outperforming fine-tuned LLMs and providing a scalable framework for organizing survey literature.

4.2.2. Section-level Related Work Generation

Section-level Related Work Generation has been regarded as a prominent research [118, 119, 583, 498, 357, 447]. Such section-level approaches are well-aligned with the actual structure of scientific papers and can effectively fulfill the requirements of the related-work-section [293].

Extractive Related Work. Early automated methods for generating the “Related Work” section involve extracting key sentences from multiple papers, which were then rewritten and combined into a coherent narrative [293]. A subsequent approach refine this by selecting papers that cited similar references to the target work and extracting relevant sentences from them [104, 792]. Further research has focused on

Methods	Model	Reference Quality		Outline Quality	Structure	Content Quality			Avg
		Input Cov.	Reference Cov.			Relevance	Coverage		
Human-Written	-	-	0.6294	87.62	-	-	-	-	-
AutoSurvey [807]	Claude-3-Haiku [24]	0.1153	0.2341	82.18	72.83	76.44	72.35	73.87	
SurveyForge [855]	Claude-3-Haiku [24]	0.2231	0.3960	86.85	73.82	79.62	75.59	76.34	
AutoSurvey [807]	GPT-4o-mini [644]	0.0665	0.2035	83.10	74.66	74.16	76.33	75.05	
SurveyForge [855]	GPT-4o-mini [644]	0.2018	0.4236	86.62	77.10	76.94	77.15	77.06	
SurveyForge [855]	DeepSeek-v3 [479]	0.2554	0.4553	87.42	79.20	80.17	81.07	80.15	

Table 2: A comparison of document-level survey generation capabilities on SurveyBench [855] using three key Survey Assessment Metrics: Reference quality, Outline quality, and Content quality. “Input Cov.” indicates the overlap between retrieved papers and benchmark references, while “Reference Cov.” evaluates the alignment of cited references with the benchmark. Data are sourced from Yan et al. [855].

improving the organization and integration of these extracted sentences. Some methods explore optimal reference structures and sentence orderings [310, 168]. For instance, ReWoS [293] and RWS-Cit [104] build topic trees to sequence sentences, while Wang et al. [812] employ a ranking mechanism based on predicted salience probabilities to enhance the quality of the extractive related work.

Generative Related Work. Recent studies have focused on methods to structure citations and generate cohesive connecting text for entire related work sections [793, 488, 448]. These approaches generally fall into three categories: **(1) Human-Guided Generation:** This approach incorporates human input, such as keywords, short abstracts, or paper groupings, to guide the generation process and maintain focus [449, 535]. For instance, Gu and Hahnloser [258] and Li et al. [450] integrate user-provided or self-extracted keywords for better related-work generation. **(2) Graph-Guided Generation:** These methods utilize citation relationships through bibliographic graphs [229, 118, 881]. Specifically, Wang et al. [812] enhance related work generation by performing random walks on heterogeneous citation graphs. Similarly, Chen et al. [119] use a graph to link references to the paper. **(3) Model-Guided Generation:** In this approach, models complete the task autonomously, without additional human input [679, 794, 606]. Guo et al. [267] and Nishimura et al. [573] treat related work generation as a summarization task with structured paragraphs and novelty statements. Additionally, Pu and Demberg [608] integrate Rhetorical Structure Theory into LoRA-based fine-tuning to identify discourse relations, and Achkar et al. [4] propose a customizable multi-stage pipeline (retrieval, citation extraction, context aggregation, polishing), further enhancing the related work generation processes.

4.2.3. Document-level Survey Generation

Document-level survey generation seeks to automate the creation of systematic literature reviews by leveraging existing research and established frameworks [819, 948, 69, 218, 830]. The detailed comparison results can be found in Table 2. For example, AutoSurvey [807] employs cue-word guidance to direct LLMs through a staged generation process. Similarly, LitLLM [7] enhances content structuring by implementing a plan-based search mechanism. SurveyX [464] strengthens logical coherence through the combination of online reference retrieval and AttributeTree preprocessing. Building on these approaches, SurveyForge [855] retrieves high-quality papers via scholar-navigating intelligences and generates survey chapters from a predefined outline, followed by iterative refinement to maintain document-level quality [699]. In contrast, STORM [676] uses multi-agent dialogue to further enhance generation performance. Beyond training-free agent management, Bio-SIEVE [645] and Susnjak et al. [734] fine-tune LLMs specifically for survey generation [405], while OpenScholar [26] offers a pipeline for training models for survey writing without relying on specialized generation architectures.

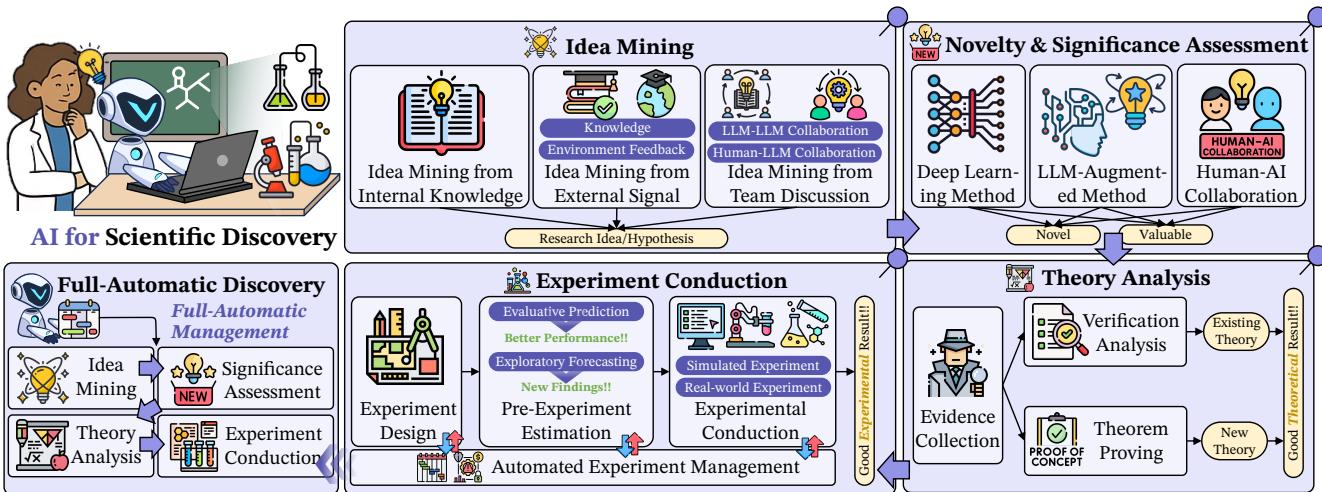


Figure 5: The AI-augmented pipeline for scientific discovery, encompassing Idea Mining, Novelty & Significance Assessment, Theory Analysis, and Experiment Conduction. Full-Automatic Discovery integrates these elements into a cohesive, end-to-end process, supporting scientific exploration and innovation.

5. AI for Scientific Discovery

AI for Scientific Discovery [783, 655, 628] leverages AI to generate novel hypotheses, theories, or ideas based on existing knowledge. Its goal is to expedite the research process by automating tasks such as idea generation, novelty and significance evaluation, theoretical analysis, and experimental design. This approach not only guides new research directions but also addresses complex scientific challenges [510, 279, 286]. As shown in Figure 5, it contains five main categories: Idea Mining (§ 5.1), Novelty & Significance Assessment (§ 5.2), Theory Analysis (§ 5.3), Experiment Conduction (§ 5.4) and Full-Automatic Discovery (§ 5.5).

5.1. Idea Mining

Idea mining, also known as hypothesis generation, is crucial for producing innovative, impactful research [577, 35, 146]. Recent studies show that the LLMs exhibit strong creativity and can facilitate automated scientific discovery [502, 398, 687, 259]. A comprehensive comparison of these findings is presented in Table 3. This suggests a future where AI agents act as independent researchers. Current efforts in this domain focus on extracting ideas from various sources to foster innovation [664, 717, 476]. These methods can be broadly categorized into three main approaches:

5.1.1. Idea Mining from Internal Knowledge

Idea mining from internal knowledge leverages the latent knowledge and generative capabilities of large language models to discover novel concepts without relying on external data [240, 687, 398]. By leveraging pretrained parameters and customized prompts, researchers can extract a variety of high-quality ideas embedded within the model [542, 105, 735]. Earlier, Meincke et al. [543] guided LLMs toward distinct “idea spaces” by adjusting decoding temperatures and applying constraint-based prompts, effectively encouraging exploration of diverse thematic trajectories. Building on these insights, Haarmann [272] conduct an empirical study where undergraduates use an interactive tool that auto-prompted GPT-4 with business-model templates, resulting in ideas with higher novelty and feasibility, all without extensive innovation training. Additionally, Liu et al. [497] demonstrate that injecting metadata into the LLM-based ideation process and applying automated validation during selection significantly increased idea feasibility and overall quality in climate-

Model	Fluency	Feasibility	Clarity	Originality	Flexibility	Average
DeepSeek-R1 [265]	6.63	6.52	8.10	7.84	6.83	7.18
Deepseek-R1-Distill-Qwen-32B [265]	7.06	6.08	7.43	7.13	6.62	6.86
Deepseek-R1-Distill-Llama-70B [265]	6.66	6.07	7.43	6.98	6.41	6.71
Claude-3.7-Sonnet [24]	7.80	5.46	7.61	7.81	6.92	7.12
Claude-3.5-Sonnet [24]	6.90	5.42	7.85	7.83	6.62	6.92
Claude-3.5-Haiku [24]	5.61	5.05	7.40	7.72	6.08	6.37
Claude-3-Opus [24]	5.74	5.66	7.72	6.66	6.04	6.36
Gemini-2.0-Flash-Exp [747]	7.30	6.02	7.84	7.37	6.83	7.18
Gemini-2.0-Flash-Thinking-Exp [747]	7.38	6.05	7.69	7.35	6.83	7.06
Gemini-2.0-Pro-Exp [747]	6.84	5.88	7.90	7.76	6.75	7.03
Gemini-Pro-1.5 [748]	6.68	5.92	7.75	7.33	6.58	6.85
GPT-4o [3]	6.12	5.58	7.74	7.64	6.38	6.69
o1-mini [336]	5.89	6.20	7.77	7.09	6.33	6.66
o1 [336]	6.23	5.88	7.42	7.23	6.29	6.61
o3-mini [336]	5.57	5.91	7.43	7.45	6.21	6.51
o3-mini-high [336]	5.76	5.82	7.62	6.95	6.17	6.47
GPT-4o-mini [3]	5.28	5.86	7.45	6.67	6.00	6.25
Llama-3.1-405B-Instruct [253]	6.57	5.56	7.48	7.18	6.33	6.62
Llama-3.1-70b-Instruct [253]	6.71	5.49	7.34	7.16	6.38	6.62
QwQ-32B [754]	6.45	6.35	7.98	7.77	6.75	7.06
QwQ-32B-Preview [753]	7.49	6.10	7.46	6.87	6.71	6.93
Qwen-2.5-72B-Instruct [857]	6.17	5.99	7.72	6.91	6.29	6.62
Qwen-2.5-7B-Instruct [857]	6.66	6.02	7.17	6.34	6.17	6.47
Mistral-Small [344]	7.36	5.97	7.36	6.98	6.62	6.86
Mistral-Large [344]	6.68	6.06	7.69	7.01	6.50	6.79
Nova-Pro-v1 [333]	6.45	6.19	7.41	6.59	6.25	6.58
Nova-Lite-v1 [333]	4.51	6.06	7.38	6.60	5.71	6.05
Phi-4 [1]	6.58	5.80	7.57	7.24	6.42	6.72
Gemma-2-27b-IT [749]	7.18	5.50	7.36	6.86	6.38	6.65
Grok-2 [841]	5.76	5.82	7.62	6.95	6.17	6.47

Table 3: Results from the Liveideabench benchmark [658] across five key dimensions: Fluency, Feasibility, Clarity, Originality, and Flexibility. Data is sourced from Ruan et al. [658]. The **bolded** contents indicate the highest performance for each metric.

negotiation experiments. Furthermore, Chen et al. [112] model the process of inference-time learning and reasoning as a circuit, enhancing the idea-mining ability of the model through various voltage-enhancing techniques.

5.1.2. Idea Mining from External Signal

LLMs in research workflows can leverage not only internal parameterized knowledge, but also external signals to generate more novel, feasible, and contextually relevant hypotheses and ideas. By incorporating structured knowledge repositories or experimental feedback, these approaches extend beyond purely internal reasoning. We categorize them into two types:

Idea Mining from External Knowledge involves supplying AI with curated academic data, such as publication metadata, citation networks, or knowledge graphs, to drive idea mining. Integrating up-to-date, domain-specific information ensures that generated hypotheses align with the latest developments in the

field [485, 442, 577]. Early efforts, limited by the capacity of earlier language models, focus on predicting relationships between concepts to generate classical “A+B” ideas [290, 387]. With recent advancements in language modeling [619, 927], attention has shifted to utilizing LLMs to explore ideas from scholarly data [528, 485]. To support this, researchers have proposed various strategies for organizing literature to optimize knowledge extraction and mining. These mainly include ternary knowledge representations [797], chained structures [435], comprehensive databases [800], and knowledge graphs [79, 260, 224]. Furthermore, efforts have focused on refining the knowledge injection process in idea mining. For example, Gu et al. [259] propose a framework with (1) a generalized retrieval system for cross-domain knowledge discovery and (2) a structured combinatorial process for improved idea mining.

Idea Mining from External Environment Feedback involves treating idea mining as an interactive loop that incorporates feedback from experimental or simulated environments [36, 609]. Static document mining, by contrast, often overlooks the complexities of the real world, limiting its potential for innovation. These methods enable AI systems to propose experiments, receive outcome data, and refine subsequent ideas, thereby mimicking the research cycle of design, execution, and analysis [29, 12]. In this domain, researchers primarily utilize multi-agent-based autonomous research systems, integrating idea mining agents with experiment conduction agents [669, 668, 332]. Furthermore, researchers have successfully extended idea mining to various experimental disciplines, including chemistry [520], materials science [568], biology [153], medicine [735, 252], and machine learning [322, 582].

5.1.3. Idea Mining from Team discussion

Idea mining from team discussion encompasses approaches that simulate or facilitate collaborative brainstorming among multiple agents, either purely algorithmic or involving human participants, leveraging iterative critique, background knowledge retrieval, and facet recombination to generate richer, more diverse idea portfolios than single-agent pipelines.

AI-AI Collaboration improves scientific ideation by refining hypotheses, critiquing proposals, and integrating external knowledge (also referred to as multi-agent collaboration) [735, 504]. We categorize current approaches into two mainstreams: (1) **Feedback-guided Mining** involves agents exchanging critiques at various research stages to refine hypotheses through iterative feedback. Some studies introduce feedback loops across idea mining, experimental design, and result interpretation to optimize performance [945, 866, 698], while others refine hypotheses using earlier outputs [308]. These methods integrate peer review [509], direct critiques of hypotheses [36], and evaluations of experimental results [521, 883]. (2) **Team-Discussion-guided Mining** assembles multiple agents with distinct roles to simulate human research team dynamics [610, 570, 234]. Specifically, Su et al. [720] create a virtual research team (VirSci) where agents iteratively propose and critique ideas, producing more novel concepts than single-agent prompts by leveraging an expanding idea archive [900, 509]. Yang et al. [867] has developed a multi-intelligentsia framework, MOOSE-Chem, based on LLMs, specialized in scientific hypothesis discovery in chemistry, which can perform the functions of retrieving inspiration and generating hypotheses based on research contexts. Moreover, Li et al. [435] introduce the Chain-of-Ideas (CoI) agent, which organizes literature into a sequential chain, mirroring a topic’s historical progression. This method generates outputs of similar quality to small research teams with minimal costs. Lagzian et al. [404] further enhance diversity and novelty via inference-time multi-view brainstorming.

Human-AI Collaboration means the process where a human researcher guides an LLM’s exploration by selecting and curating intermediate artifacts, which the model then recombines and refines [569, 568]. For instance, Radensky et al. [626] introduce Scideator, a system that enables researchers to select various facets, such as the problem statement, methodology, and dataset, from existing papers. The LLM subsequently

recombines these facets to generate novel candidate ideas, significantly improving the idea qualities. Similarly, Garikaparthi et al. [228] present IRIS, an interactive research ideation system that facilitates human-AI collaboration by validating research motivations and synthesizing methodological suggestions in response to researcher queries. However, the research findings [396] show that, although LLM assistance can yield short-term boosts in creativity during supported tasks, it may inadvertently hamper users' independent creative performance when working unassisted, thereby raising concerns about its long-term effects on human creativity and cognitive abilities.

5.2. Novelty & Significance Assessment

Novelty & Significance Assessment focuses on AI methods that evaluate the originality and impact of ideas and scholarly papers [353, 687, 372]. The field predominantly employs three approaches: **(1) Traditional Methods:** Initially, models are trained to classify or regressively assess novelty and significance [179, 331, 806]. For instance, Singh and Chakrabarti [692] propose SAPPhIRE that utilizes the causality ontology to quantify novelty in design problems, measuring textual similarity at multiple abstraction levels against historical works. Additionally, Wang [782] introduce “surprise” as an alternative measure of novelty, comparing a paper’s word distribution to a language model’s representation of scholarly discourse. This approach aligns with scientific intuition (face validity) and shows a correlation with expert judgments (construct validity). **(2) LLM-Augmented Methods:** With the significant development of LLMs, a series of works try to integrate LLMs for better novelty and significance assessment [836]. Typically, Feng et al. [207] propose GraphEval, a lightweight, graph-based LLM framework for reasoning evaluation, that prompts a small-scale LLM to decompose complex reasoning processes into easily interpretable “viewpoint” nodes, thereby enhancing the robustness of reasoning assessment. **(3) Human-AI Collaboration Methods:** Unfortunately, purely LLM-augmented assessments of novelty may overestimate creativity [93, 414] and lead to homogenization effects without human input [21, 946]. As a result, there is growing interest in human-AI collaboration for novelty assessment, with several works [27, 501, 586] advocating for the integration of human-guided ideation alongside LLM-based workflows.

5.3. Theory Analysis

Any scientific idea or hypothesis must be rigorously evaluated to confirm its validity. Theory analysis involves using AI methods to determine whether a hypothesis aligns with established scientific principles. AI applications in theory analysis can be divided into three main components:

5.3.1. Scientific Claim Formalization

Scientific claim formalization converts natural-language assertions into structured representations for systematic verification [636, 399, 549]. Early approaches relied on template-based methods [250]. For example, Heger et al. [288] describe a pipeline that converts complex hypotheses into machine-readable templates. Subsequent works focus on incorporating LLMs to refine these templates. Ganguly et al. [221] propose a PCFG-based framework to address common LLM failure modes, while Valsci [185] automates the conversion of natural-language claims into templated queries for LLM-driven verification. More recently, Yan et al. [856] suggest that integrating text, images, and other modalities in multimodal LLMs provides richer structured representations, facilitating cross-domain reasoning.

5.3.2. Scientific Evidence Collection

Scientific evidence collection involves systematically identifying, retrieving, and curating data sources to support or challenge research claims [589, 771, 370]. Previous studies have focused on methods for

evaluating and improving the quality of retrieved sources [768] and optimizing retrieval configurations [769]. Additionally, strategies have emerged to address incomplete or faulty evidence, including techniques for detecting missing information [242] and understanding the causes of retrieval errors [840, 243]. More recent efforts have integrated LLMs with retrieval systems to enhance the accuracy of evidence retrieval and verification. For instance, SciClaims [580] combines claim extraction, evidence retrieval, and verification into a single LLM-powered pipeline, streamlining the entire process. Similarly, Alvarez et al. [17] and Wang et al. [799] extend retrieval-augmented generation by producing structured query representations and retrieving corroborating or refuting evidence in a single step.

5.3.3. Scientific Verification Analysis

Scientific verification analysis plays a critical role in AI-driven theoretical qualitative studies by assessing the logical coherence [392, 462], factual consistency [556, 365, 91, 75], and robustness [337] of claims based on existing evidence. Research underscores the importance of domain expertise for accurate and reliable verification [162, 16, 50, 839]. To mitigate errors and enhance interpretability, some frameworks adopt human-like, stepwise pipelines [378, 157, 831, 30]. For instance, HiSS [911] and ProToCo [891] employ multiple cueing to validate each substatement, improving reliability. Other methods integrate verification with experimental results to boost transparency and interpretability [389, 588, 190, 908]. GX-Chen et al. [271] show that LLMs inherit reasoning heuristics from training data, leading to cognitive biases. To mitigate this, they propose an inference-time-scaling sampling procedure that reduces implicit causal assumptions and aligns the model's reasoning with causal rigor. More recently, Ku et al. [392] introduced the task of generating coherent visual explanations and demonstrated that combining agents with Manim animations to produce long-form theorem explanation videos (over five minutes) results in more effective visual explanations.

5.3.4. Theorem Proving

Theorem proving involves the development of algorithms and models, often incorporating generative language models, to autonomously generate and verify formal mathematical proofs [456, 215, 947, 859]. Early methods [780, 409] introduce dynamic tree proof search techniques and integrate retrieval algorithms with language models for theorem proving [602]. However, retrieval algorithms tend to prioritize trivial intermediate conjectures, resulting in poor performance [781]. To overcome this, some researchers have introduced novel approaches that replace retrieval algorithms entirely [343, 342]. LEGO-Prover [779] employs Growing Libraries to enhance LLM reasoning, while Zhao et al. [930] suggest Subgoal-based Demonstration Learning for more effective theorem proving. Additionally, Lean Copilot [706] and Lean-STaR [470] leverage the Lean programming language and theorem prover to enable improved human-AI collaboration in proof completion. Recent studies have focused on fine-tuning specialized proving LLMs [211]. For example, MUSTARD [325] and DeepSeek-Prover [846] aim to generate high-quality synthetic data to fine-tune models and improve theorem proving.

5.4. Scientific Experiment Conduction

Automatic Scientific Experiment Conduction leverages AI to design, conduct, and analyze scientific studies autonomously, aiming to automate the entire process, from hypothesis formulation to data interpretation. This automation seeks to accelerate research and improve reproducibility [113, 385, 49, 767]. However, Zhu et al. [951] highlight a critical challenge: AI scientists currently lack the validation capabilities needed for rigorous experimentation and high-quality manuscript production. Without these essential competencies, such platforms cannot succeed.

5.4.1. Experiment Design

Experimental design is vital for efficiency and provides the foundation for AI-assisted experiment conduction methods [767, 153, 252, 234]. Evidence shows that systematic design plays a central role in automating and enhancing experimental processes [568, 520].

Semi-Automatic Experiment Design involves the creation of experimental plans through human-AI collaboration [568, 520]. Arlt et al. [25] present a transformer-based framework that autonomously generates quantum experiment protocols and uncovers state preparation principles. Huang et al. [324] integrate deep learning with multi-objective optimization to design polymer sequences with both high thermal conductivity and synthetic feasibility, validating their results through molecular dynamics. Liang [461] apply a variational autoencoder combined with reinforcement learning to enhance the design and efficiency of parameters for cultural creative products. Craig [150] propose a human-AI collaboration framework based on experimental design, case-based reasoning, and a note-taking system, offering scientists a structured LLM tool with transparent documentation, resulting in verifiable experimental designs and knowledge integration.

Full-Automatic Experiment Design refers to the application of agent-centric methods for the automatic scheduling of scientific experiments [332, 12, 236]. Platforms such as The AI Scientist [509] and Agent Laboratory [669] continuously refine experimental protocols by incorporating new data in real-time [735, 36, 668]. In a significant development, Liu et al. [487] proposed an end-to-end generative-agent framework that enables fully autonomous planning, spanning from literature review to protocol iteration, without the need for human intervention. Additionally, Roohani et al. [651] introduced a biodiscovery agent capable of designing, evaluating, and optimizing gene-perturbation experiments. This system has shown superior performance over traditional Bayesian methods, especially in targeting non-essential genes.

5.4.2. Pre-Experiment Estimation

Pre-experiment prediction leverages AI to forecast experimental outcomes, aiming to improve research efficiency and accuracy. This process can be divided into two categories:

Evaluative Prediction predicts quantitative values or trends of experimental outcomes, such as estimating drug concentration effects, determining whether a compound affects cellular activity, and assessing protocol feasibility [153]. **(1) Deep-Learning Methods:** With the rise of deep learning, hierarchical prediction models have emerged [838]. Li et al. [439] incorporated physical equations to predict pharmacokinetic parameters, reducing data requirements and enhancing noise robustness. More recently, Li et al. [440] proposed a dual-matching framework, combining hierarchical molecular alignment with meta-learning, which showed significant improvements in drug feature estimation. **(2) LLM-Augmented Methods:** More recently, with the advent of LLM capabilities, Zhang et al. [909] demonstrate successful LLM-assisted evaluative prediction, a method that has been further extended in subsequent studies. Notably, Luo et al. [517] integrate BrainGPT into neuroscience literature retrieval, outperforming domain experts in evaluating experimental estimation. Wen et al. [822] develop a system combining fine-tuned GPT-4.1 with a paper retrieval agent, which outperformed 25 human experts in evaluating experimental predictions.

Exploratory Forecasting utilizes AI to predict experimental outcomes, generate new compounds, design reaction pathways, and propose combinatorial schemes to drive scientific discovery [520, 496]. Several studies have applied deep generative models for chemical-space forecasting [247, 165]. Seo et al. [672] introduce a framework that uses graph diffusion modeling to predict ingredient-chemical molecule interactions, enabling innovative pairing exploration. Furthermore, based on a massive computation model, DeepMind's GNoME [41] predicts approximately 380,000 stable material structures, demonstrating AI's potential in materials discovery. Recently, multi-turn interactive methods have also been developed to improve exploratory

forecasting [252]. For instance, Zhang et al. [909] and Swanson et al. [735] present platforms that integrate multi-agent debates to better forecast experimental performance and foster idea exchange, advancing the discovery of new method variants.

5.4.3. *Experiment Management*

The integration of machine learning and robotics in AI-driven experiment management enables hypothesis generation, high-throughput experimentation, and iterative procedure refinement without human intervention [44, 675, 933, 23]. These paradigms, also named as “self-driving laboratories” [76, 87, 283], promise accelerated discoveries [201] in biology, chemistry, and materials science [402, 89, 200].

Open-Loop Management involves experimental management without human oversight [775]. Hysmith et al. [328] explore human-AI collaboration, emphasizing the interoperability of robots, predictive models, and data pipelines. In bioprocessing, Zournas et al. [960] combine active learning with a semi-automated Design-Build-Test-Learn cycle to optimize microbial media, showing that higher NaCl levels significantly improve metabolite yield and process efficiency. Google DeepMind and BioNTech [210] have introduced an AI-driven laboratory assistant to autonomously design protocols and predict outcomes, aiming to enhance research efficiency in the medical, energy, and educational sectors. Reports indicate that such systems could reduce the traditional 20-year, \$100 million timeline for materials discovery to just months. The U.S. government is supporting these efforts through strategic funding initiatives [33].

Close-Loop Management entails fully autonomous experimental management without human intervention [775]. The Functional Genomics Explorer [381] is a landmark in this area, being the first fully autonomous research platform that generates hypotheses, designs experiments, and validates results. MacLeod et al. [526] describe a robotic system that formulates, deposits, and characterizes thin films using model-based optimization to enhance charge transport. AI-driven optimization algorithms are transforming experimental workflows, as seen in closed-loop Bayesian optimization methods for chemical and materials discovery [759]. Knox et al. [383] apply multi-objective optimization to polymer nanoparticle synthesis, optimizing size, dispersity, and functionality.

5.4.4. *Experiment Conduction*

Experiment conduction refers to the application of AI techniques in executing and managing scientific experiments. This process is essential for automating workflows, ensuring experiments are carried out efficiently and accurately. The primary aim of experiment conduction is to reduce human involvement in the experimental process. It can be further divided into two categories:

Automated Machine Learning Experiment Conduction uses AI to streamline the design, training, and evaluation of ML models, reducing dependence on human expertise by covering the entire pipeline from preprocessing to hyperparameter optimization [905, 761, 256, 919, 576, 937]. Typically, Wang et al. [804] present a community-driven sandbox allowing agents to write code, browse the web, and coordinate through an event-stream API. For Kaggle challenges, Li et al. [459] propose an iterative, collaborative multi-agent system that incorporates debugging and unit testing across the competition pipeline. AIDE [176] utilizes a tree-search loop to generate, evaluate, and refine solutions, achieving a bronze medal in Kaggle competitions. At the research level, Li et al. [443] formalize a three-phase LLM agent workflow, idea generation, implementation, and execution, to automate experiments. Zhao et al. [929] and Liu et al. [483] present a multi-agent method for extracting model variables from scientific texts, significantly improving experimental reproduction accuracy. Cheng et al. [129] introduce a multi-agent framework for crafting novel LLMs by emulating standard research stages and leveraging scaling laws through a “Ladder of Scales”.

Models	Without Knowledge				With Knowledge			
	SR	CBS	VER	Cost ↓	SR	CBS	VER	Cost ↓
<i>Direct Prompting</i>								
Llama-3.1-Instruct-70B [253]	5.9	81.5	29.4	0.001	4.9	82.1	27.5	0.001
Llama-3.1-Instruct-405B [253]	3.9	79.4	35.3	0.010	2.9	81.5	25.5	0.001
Mistral-Large-2 [344]	13.7	82.3	47.1	0.009	16.7	84.7	39.2	0.001
GPT-4o [3]	11.8	82.6	52.9	0.011	10.8	83.8	41.2	0.016
Claude-3.5-Sonnet [24]	17.7	83.6	51.0	0.017	21.6	85.4	41.2	0.016
o1-preview	34.3	87.1	70.6	0.221	31.4	87.4	63.7	0.236
<i>OpenHands CodeAct [805]</i>								
Llama-3.1-Instruct-70B [253]	6.9	63.5	30.4	0.145	2.9	65.7	25.5	0.252
Llama-3.1-Instruct-405B [253]	5.9	65.3	32.0	0.383	8.3	71.4	58.0	0.384
Mistral-Large-2 [344]	9.8	72.5	53.9	0.513	13.7	78.8	50.0	0.759
GPT-4o [3]	19.6	83.4	87.5	0.803	27.5	86.3	73.5	1.094
Claude-3.5-Sonnet [24]	21.6	83.6	87.3	0.958	24.5	85.1	88.2	0.900
o1-preview [336]	33.4	86.2	87.0	0.999	35.3	88.4	91.5	0.913
<i>Self-Debug [117]</i>								
Llama-3.1-Instruct-70B	13.7	82.7	40.4	0.007	16.7	83.5	73.5	0.005
Llama-3.1-Instruct-405B	16.7	80.0	35.3	0.006	23.6	79.4	40.4	0.004
Mistral-Large-2 [344]	23.5	85.1	78.4	0.007	26.5	86.7	84.3	0.006
GPT-4o [3]	22.6	84.4	84.3	0.024	33.4	87.1	86.3	0.037
Claude-3.5-Sonnet [24]	32.4	86.4	92.2	0.026	34.5	87.1	86.3	0.015
o1-preview [336]	42.2	88.4	92.0	0.636	41.2	88.9	91.2	0.713

Table 4: Full-automatic discovery capability comparison on ScienceAgentBench [127]. The data presented are derived from Chen et al. [127]. The **bolded** contents indicate the highest performance for each metric.

Designs are proposed, adversarially reviewed, implemented, and evaluated across model sizes from 14 million to 350 million parameters.

Real-world Experimental Simulation & Conduction. Recent advancements in the planning and reasoning capabilities of LLMs have led to their use in simulating experimental results [359, 889, 416, 888] and even direct conduct real-world experiments [123, 659, 203]. Real-world experimental simulation & conduction generally employ four strategies: **(1) Self-Improvement:** Models iteratively refine their performance based on feedback [313, 683, 916, 596, 883]. For example, Siddiqui et al. [688] enhance functional approximation through iterative knowledge application. Further refinement occurs through analytical insights [443, 737, 36] and hyperparameter tuning [568, 494, 901]. **(2) Multi-Agent Interaction:** Models simulate collaborative research teams by assigning roles such as experimenter, analyst, or critic [36, 234, 713, 307, 702]. For instance, MechAgent [567], Researchcodeagent [219] and The AI Scientist [509, 854] automate experiments through multi-agent collaboration, with LLMs acting as proxies in fields like computer science [509, 854], social science [552, 532], and physical science [906]. **(3) External Tool Integration:** Researchers enhance model capabilities by linking them to databases, APIs, and other tools during experiments [278, 621, 666]. For example, Boiko et al. [68] integrate internet search, code execution, and automation into a GPT-4 system. Studies like ChemCrow [520] and Crispr-GPT [316] support chemistry and gene editing experiments through massive specialized toolchains. **(4) Specific Fine-Tuning:** A growing body of work explores the fine-tuning of specific models to improve experimental simulations. For instance, Cui et al. [152] present a transformer-based model trained on large single-cell transcriptomic datasets, achieving state-of-the-art accuracy in cell-type annotation and in silico perturbation response [491].

5.4.5. Experimental Analysis

Experimental Analysis involves systematically testing hypotheses, evaluating models, or validating theoretical assumptions to draw meaningful conclusions. This process encompasses three main sub-processes:

Automated Evaluation Metrics refer to systems like AutoML that automatically generate model learning curves, parameter sensitivity analysis graphs, and other evaluation tools to assess model performance [5]. For instance, AutoML platforms assist researchers by automatically producing learning curves and sensitivity analysis graphs to better understand model behavior [42, 40].

Theoretical Consistency Analysis ensures that the theoretical methods align with the experimental implementations [483]. AutoReproduce [929] uses a large language model to create a multi-intelligent body system, enabling automatic comprehension, code reproduction, and execution verification of experiments in scientific papers. This process completes the consistency analysis between theoretical methods and experimental outcomes.

Exploratory Analysis is essential for investigating and understanding datasets through statistical and visualization techniques to identify patterns, spot anomalies, test assumptions, or validate hypotheses [101, 722]. This process extends the capabilities of language models for data exploration in structured formats. For example, Xing et al. [847] utilizes a generator-validator fine-tuning approach to enable language models to specialize in parsing tabular data, improving table structure inference and summarization. Additionally, Bian et al. [62] developed HeLM, which facilitates high-quality natural language summarization of table content, aiding in the generation of conclusions.

5.5. Full-Automatic Discovery

Full-automatic discovery refers to the ability to close the loop of the scientific process, from hypothesis generation and experimental design to autonomous execution, result analysis, and iterative feedback, powered by end-to-end artificial intelligence [531]. A comprehensive comparison of the results is presented in Table 4. Advances in laboratory automation and closed-loop assistants are driving fully automated discovery toward greater reliability, innovation, and faster iteration through multi-agent systems [560, 563, 752, 332]. For example, Lu et al. [509] and Yuan et al. [883] use literature mining to rank research topics, employ an “anomaly-guided” code-synthesis framework to generate and debug experimental scripts, and feed results back into the ideation module to iteratively refine hypotheses [669, 668, 540]. Kon et al. [384] introduce rigor through three modules: intra-agent rigor for reliability, inter-agent rigor for systematic control, and an experimental knowledge module for interpretability, addressing issues of insufficient rigor and overstated claims. Li et al. [453] extend this approach to data-driven discovery, enhancing exploration diversity. Further, Zochi [12] is developed as an AI-driven system for end-to-end scientific discovery, demonstrating its comprehensive capabilities across the research lifecycle. Papers generated through Zochi have even been accepted by ACL 2025.

6. AI for Academic Writing

AI for Academic writing involves the use of AI techniques to assist researchers or generate from scratch in drafting, editing, and formatting scientific manuscripts [373]. With the development of deeper interaction between human and LLMs, human and LLMs are quickly shaping each other’s better writing habits [230, 86, 943]. As shown in Figure 6, it contains two main categories: Semi-Automatic Academic Writing (§ 6.1) and Full-Automatic Academic Writing (§ 6.2).

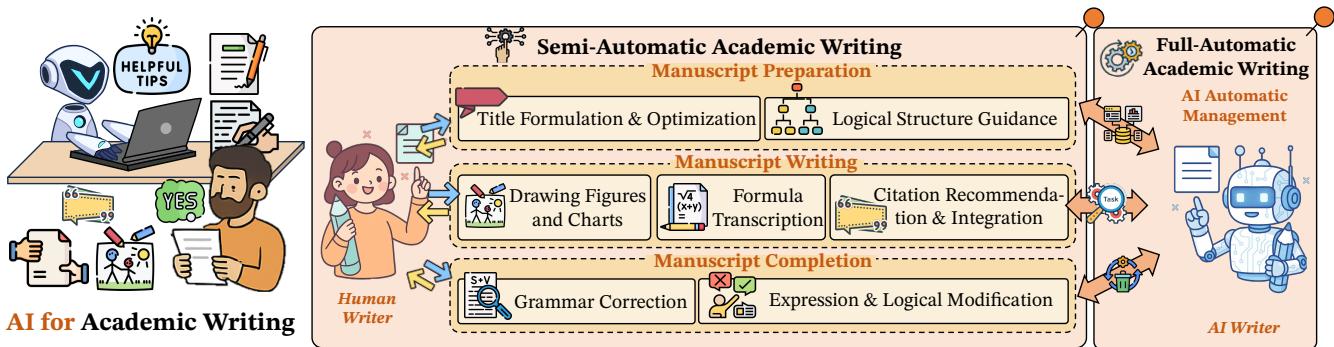


Figure 6: The main paradigms of AI for Academic Writing. It can be divided into two main categories: Semi-Automatic Academic Writing and Full-Automatic Academic Writing. Specifically, Semi-Automatic Academic Writing encompasses Manuscript Preparation, Manuscript Writing, and Manuscript Completion.

6.1. Semi-Automatic Academic Writing

Semi-automatic academic writing involves the use of AI tools to assist researchers in drafting and editing scientific manuscripts, requiring human input and oversight. This approach aims to enhance the quality and efficiency of scientific writing by offering AI-generated suggestions, corrections, and formatting assistance. Semi-automatic academic writing can be categorized into three phases:

6.1.1. Assistance During Manuscript Preparation

Assistance During Manuscript Preparation refers to the support provided by models and tools throughout the manuscript creation process. This includes generating and refining titles, guiding the overall structure, and ensuring content coherence, all aimed at improving the clarity, quality, and readiness for submission.

Title Formulation and Optimization involves using models to generate multiple title candidates and selecting the most suitable one [72, 63]. For example, given a research topic like “new energy battery materials”, a model generates 5-10 titles with varying focuses, which are evaluated based on novelty, complexity, and potential impact, helping the author select the best option [63]. To further improve the title quality, Rehman et al. [641] fine-tune PEGASUS-large and use GPT-3.5-turbo (zero-shot) to generate titles from abstracts. Au et al. [31] enhance title quality by incorporating user preferences for more coherent and personalized titles.

Overall Logical Structure Guidance involves providing the model with section and subsection headings, as well as paragraph outlines, to evaluate the logical flow, ensure the avoidance of repetition, correct ordering errors, and identify any missing elements [281]. Sun et al. [725] propose a multi-stage workflow for assessing paper structure. Their rubric emphasizes the importance of section completeness and content cohesion, ensuring that headings and paragraphs adhere to established formatting standards.

6.1.2. Assistance During Manuscript Writing

Semi-automatic AI writing involves a collaborative process where humans create the primary content, while AI contributes supplementary elements. In this collaboration, AI assists with tasks that are secondary to the main content [468, 128, 852, 704, 566]. This process can be divided into three primary tasks:

Drawing Figures and Charts serves as an effective means of conveying experimental data and analysis [55, 97]. Recent advancements in AI research on automatic scientific figure generation have led to significant

breakthroughs [902, 295, 750, 638]. Rodriguez et al. [646] introduce the FigGen model, which maps textual descriptions to complex academic figures with high fidelity. Beyond direct image generation, several studies have explored programming scientific diagrams using Python [928, 921, 133, 553], SVG [648], or tikz [55, 54] for better figure quality. However, figures alone cannot fully convey results; captions are essential for ensuring that readers understand each figure [90, 509, 873]. To address this, Hsu et al. [302] develop SciCapenter, an interactive system that generates multiple caption candidates, scores them, and quality-checks each, assisting authors in selecting the most optimal phrasing. MLBCAP [377] utilize multiple LLMs to collaborate on chart-based title generation. Additionally, frameworks like AI Scientist [509, 854] can identify key data from experimental logs, generate figures with captions, and integrate them into authoring tools, advancing end-to-end AI-driven scientific visualization.

Formula Transcription need to digitize extensive mathematical formulas and tables in academic and instructional materials, driven the development of automated tools that convert handwritten or image-based expressions into editable LaTeX. Specifically, Sundararaj et al. [732] employ a Vision Transformer (ViT) to transcribe these expressions into LaTeX, improving accuracy and reducing manual proofreading. Vrečar et al. [770] introduce a semi-automated tool for semantic annotation, enhancing the accessibility and interoperability of mathematical symbols in LaTeX. Jiang et al. [345] propose the iterative refinement framework, which generates an initial LaTeX draft, compares it to the source image for feedback, and iteratively corrects errors, thereby minimizing manual verification and facilitating better transcription.

Citation Recommendation & Integration has emerged as a key research area in academic writing, focusing on retrieving and incorporating relevant literature into documents to enhance writing efficiency and citation accuracy [914, 527, 818, 451, 14, 467]. Earlier, Ma et al. [523] introduce a temporal preference model for ranking citations, setting the stage for subsequent research considering time factors [656]. In generative models, Çelik and Tekir [92] develop CiteBART, which masks citation markers in context and reconstructs them, enabling zero-shot citation generation. More recently, Wang et al. [813] introduce ScholarCopilot, which generates special retrieval tokens and dynamically queries literature databases to embed references in real time. He et al. [287] propose PaSa, an advanced paper-search agent powered by large language models. PaSa autonomously invokes search tools, reviews manuscripts, and selects relevant references, achieving results that surpass even Google + GPT-4o in complex scholarly queries.

6.1.3. Assistance After Manuscript Completion

After completing the paper, the author typically needs to refine its quality, focusing on language accuracy and logical coherence. At this stage, support tools can assist in grammar correction, expression and logical revision, ensuring the paper is clear, fluent, and logically sound.

Grammar Correction means the model proofreads each paragraph, identifies spelling errors, improper punctuation, repetitive phrasing, and character-encoding issues, and provides corresponding revision suggestions [231, 860, 809, 724]. Specifically, Wang et al. [810] propose a synthetic data construction method based on contextual augmentation, which can ensure an efficient augmentation of the original data with a more consistent error distribution. Wang et al. [787] propose an integrated automated writing evaluation system with grammatical error correction to support L2 essay writers by providing immediate feedback, offering targeted guidance to improve grammar and coherence, reducing manual grading efforts. Further, Zheng and Zhang [940] present a Transformer-based feedback framework that generates real-time suggestions on grammar, vocabulary, sentence structure, and logical coherence for non-native English writers. Its modular design and dynamic parameter adjustment enable personalized learning paths while ensuring low-latency feedback and differential privacy.

Expression & Logical Revision highlights AI systems' role in refining scientific manuscripts post-initial draft, focusing on expression and logic [940]. (1) **Self-guided Revision** involves AI autonomously analyzing drafts and suggesting edits to improve language, cohesion, and structure [705, 199]. Ito et al. [335] propose sentence-level edits, adjusting or rewriting sentences based on draft content. Additionally, Botha et al. [73] use revision histories to segment and rewrite the text, further enhancing revision quality. (2) **Human-guided Revision** refers to interactive systems where users provide specific instructions or highlight sections for the AI to modify, forming a collaborative editing process [585, 232, 418, 558]. Faltungs et al. [191] develop an interactive editor that responds to user commands. Wordcraft [145] supports few-shot learning and dialogue for interaction. However, these methods struggle to capture the diversity and iterative nature of revision. XtraGPT [107] provides open-source LLMs for context-aware, instruction-guided revisions, addressing surface-level and section-level coherence. (3) **Human-in-loop Revision** emphasizes a cyclical workflow combining AI suggestions, human evaluation, and document updates through multiple optimization loops [205, 330, 745, 559]. Du et al. [182] propose a human-in-the-loop system that integrates model-generated edits, user feedback, and document updates for high-quality revisions [764]. Lin [478] shows that human-AI frameworks improve collaborative efficiency. Wen et al. [821] develop OverleafCopilot, a browser extension integrating LLMs into Overleaf for real-time suggestions, automatic rewriting, translation, and prompt sharing through PromptGenius to enhance LaTeX writing.

6.2. Full-Automatic Academic Writing

Full-automatic academic writing refers to using AI to generate complete scientific manuscripts without human intervention. This process spans drafting, formatting, and producing high-quality papers ready for submission, effectively removing the need for human input in manuscript preparation [790, 849]. Recent research has primarily adopted multi-agent, modular designs with self-feedback mechanisms for iterative refinement. The AI Scientist [509] treats writing and reviewing as pipeline modules: by simulating peer review and providing score-based feedback, it refines drafts. Yamada et al. [854] extend this system by incorporating vision-language model feedback loops to improve both content and figure presentation. Agent Laboratory [669, 668] employs a paper-solver module with role-based agents that simulate lab workflows, evaluate drafts against NeurIPS criteria, and iteratively enhance them. Zochi [12] uses a multi-agent architecture for initial draft generation, combining automated review with self-feedback for further polishing. Despite these successes, including some papers passing human peer review, no system has yet fully eliminated human editing, especially regarding correct citation use [332, 12, 669].

7. AI for Academic Peer Reviewing

Peer reviewing plays a crucial role in enhancing the quality of academic papers. However, it is often hindered by delays, time demands, and growing academic workloads [471, 386, 756, 956]. To address these challenges and improve dissertation quality, researchers are exploring the integration of AI into the review process [886, 492, 575, 401, 525]. As shown in Figure 7, it contains three main categories: Pre-Review (§ 7.1), In-Review (§ 7.2) and Post-Review (§ 7.3).

7.1. Pre-Review

In this phase, editors or track chairs are tasked with preliminary scoring, identifying the manuscript's subject domain, and assigning appropriate reviewers to ensure review quality and prevent conflicts of interest.

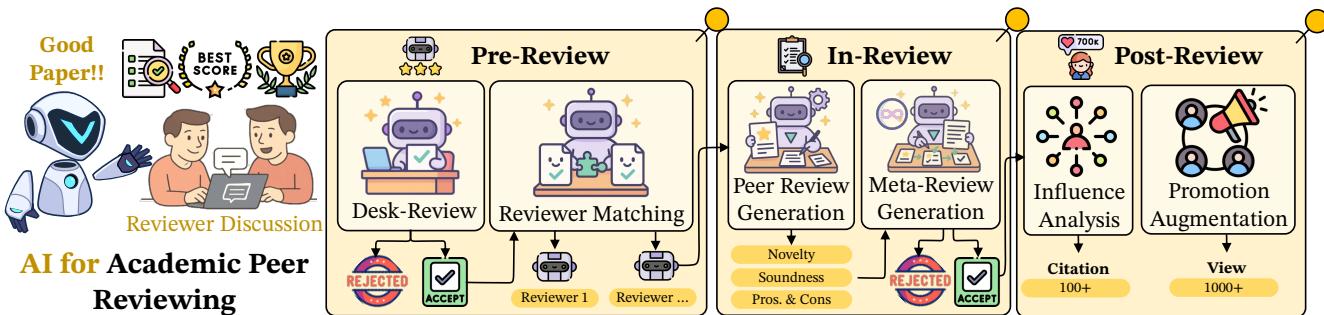


Figure 7: The primary process pipelines in AI for Academic Peer Review, encompassing three key stages: (1) Pre-Review, including Desk-Review and Reviewer Matching to ensure higher quality and more efficient evaluations; (2) In-Review, comprising Peer Review and Meta-Review, aimed at providing comprehensive scholar feedback and evaluation; and (3) Post-Review, featuring Influence Analysis and Promotion Augmentation, designed to assess the impact of the review process and improve the dissemination of scholarly work.

7.1.1. Desk-Review

As manuscript submissions to academic journals increase, editorial offices face heavier workloads during the desk-review stage. To address this, major publishers have introduced AI-driven tools, such as automated keyword extraction, topic matching, and preliminary scoring, to enhance efficiency, shorten turnaround times, and reduce manual screening [178, 428, 198]. For example, Elsevier’s Evise and Editorial Manager (EM) systems use indexing and extract terms to route manuscripts to the appropriate subject areas and editorial teams [755]. Similarly, IEEE’s Manuscript Central (built on ScholarOne) combines metadata, author-provided keywords, and an academic-network reviewer discovery tool for more accurate matching [701]. Springer’s SNAPP system and Nature’s AI-assisted triage tool also demonstrate AI’s impact on desk-review workflows [562]. Additionally, Díaz et al. [171] develop AnnotateGPT, which generates annotations to help editors quickly assess a manuscript’s scope and quality, further speeding up the review process.

7.1.2. Reviewer Matching

Reviewer matching in peer review assigns manuscripts to experts whose knowledge aligns with the submission, aiming to maximize review quality, fairness, and workload balance [595]. Charlin et al. [100] first formulate this as an integer program, using affinity scores to balance quality, fairness, and load. Charlin and Zemel [99] later embed papers and reviewer profiles in a shared latent topic space, improving efficiency and accuracy in large conferences. As submission volumes increased, automated conflict-of-interest (COI) detection became essential. Wu et al. [835] introduce a semi-automated COI declaration system and a supervised ranking model to flag conflicts and ensure fairness. Pradhan et al. [603] further advance this with a greedy algorithm that optimizes expertise distribution and workload while maintaining COI constraints, enhancing both fairness and efficiency. To address growing demands, Leyton-Brown et al. [428] develop the Large Conference Matching (LCM) algorithm, balancing expertise and load across thousands of papers. Fu et al. [217] and Aitymbetov and Zorbas [13] tackle interdisciplinary submissions by forming multidisciplinary reviewer teams to improve review quality.

7.2. In-Review

This stage involves generating or supporting review reports, either through automation or human reviewer assistance. Reviewers must assign a numerical score and provide a written evaluation. The in-review process typically involves two main stages: Peer-Review and Meta-Review.

Model	Focus similarity				Text similarity		
	KL Divergence	Overall F1	Strength F1	Weakness F1	ROUGE-L	BERTScore	BLEU-4
GPT-4o-mini [644]	0.081	0.344	0.335	0.353	0.197	0.883	0.076
GPT-4o [644]	0.082	0.348	0.342	0.354	0.202	0.885	0.079
o1-mini [336]	0.090	0.359	0.331	0.385	0.179	0.878	0.059
o1 [336]	0.097	0.355	0.318	0.388	0.170	0.869	0.032
DeepSeek-R1 [265]	0.120	0.373	0.341	0.400	0.156	0.874	0.045
Llama-3.1-70B [253]	0.136	0.339	0.338	0.341	0.215	0.882	0.076
Llama-3.1-405B [253]	0.145	0.349	0.349	0.350	0.218	0.884	0.089
DeepSeek-V3 [479]	0.151	0.350	0.330	0.368	0.199	0.880	0.069
GPT-4o-Finetuned [644]	0.022	0.306	0.280	0.322	0.194	0.882	0.081
MARG [159]	0.113	0.346	–	0.346	0.160	0.854	0.011

Table 5: Comparison of expert and LLM review performance sourced from Shin et al. [682], where “GPT-4o-Finetuned” refers to GPT-4o finetuned with review data using the finetune-API. KL divergences are calculated from the average of four focus distributions (strength/target, weakness/target, strength/aspect, weakness/aspect) between expert and LLM reviews. F1 scores for overall performance, strength, and weakness are derived by comparing the (target, aspect) sets between expert and LLM reviews. Text similarity metrics are computed to assess the alignment between LLM and expert reviews. The **bolded** contents indicate the highest performance for each metric.

7.2.1. Peer-Review Generation

Peer-review generation involves the automatic creation or assistance in the development of review comments for submitted manuscripts, including predicting quality scores and providing textual feedback. A detailed comparison of these findings is presented in Table 5.

Score Prediction estimates scores on criteria like innovation and clarity, assessing overall quality through multiple feature points [58]. Jia et al. [341] introduce a multi-task BERT framework that jointly detects quality features (e.g., suggestions, problem mentions) in review comments, outperforming single-task baselines. RelevAI-Reviewer [149] treats review tasks as a classification problem to predict papers’ relevance to a given call. Basuki and Tsuchiya [45] frame score prediction as a regression task using internal paper features, excelling at distinguishing “good” from “poor” submissions. To tackle data scarcity, Muangkammuen et al. [555] improve upon this method by introducing a semi-supervised approach that fine-tunes a transformer-based model using unlabeled data, effectively utilizing contextual cues.

Comment Generation involves generating natural-language review comments, which is the core element of manuscript evaluation [879]. Robertson [644] demonstrate that GPT-4 can generate plausible review comments. Yuan and Liu [885] construct concept graphs and integrate citation mapping on a pre-trained model to generate comments. AI-Scientist [509, 854] found that LLM-based agents approach human-level review performance [463]. MARG [159] assigns paper sections to multiple LLM agents for internal discussion, improving feedback relevance. Chamoun et al. [94] allocate four specialized roles to enhance specificity and comprehension. Furthermore, AgentReview [351] and Tan et al. [742] model the review process as a dynamic, multi-round dialogue.

Unified Generation integrates textual comments and numeric scores into a single review output that mirrors real-world peer review workflows [681, 417]. There are three main paradigms for optimizing unified peer-review generation: **(1) Single-Agent Optimization:** A straightforward approach is to optimize a single

agent through deeper analysis [360, 950, 329]. Shin et al. [682] observe that, by comparing the focus distributions of LLMs and human experts, off-the-shelf LLMs tend to prioritize technical validity in paper reviews while underemphasizing novelty. To address this, Tyser et al. [765] enhance the review system with a suite of review documents to reduce risks of misuse, score inflation, overconfident assessments, and uneven distributions. Additionally, Zhu et al. [950], Zhang and Abernethy [907] incorporate deeper reasoning via reasoning LLMs to improve review quality. **(2) Iterative Refinement Optimization:** High-quality feedback is often ensured through hierarchical quality control and multi-round refinement loops [59]. Wu et al. [833] propose an LLM-driven pipeline with hierarchical verification, producing literature surveys that match human-authored reviews. Kirtani et al. [382] introduce standardized evaluation metrics and a self-refinement cycle to align LLM-generated reviews with human accuracy and analytical depth. **(3) Multi-Agent Optimization:** To further enhance feedback reliability, some studies adopt multi-agent frameworks [742, 323, 223, 572, 851]. D'Arcy et al. [159] divide manuscripts into modules for specialized agents, leading to higher-quality feedback than single-agent systems. CycleResearcher [825] and TreeReview [98] apply reinforcement learning to simulate iterative review rounds and structured agent interactions, enhancing collaboration. Furthermore, Taechoyotin and Acuna [738] propose multi-objective reinforcement learning to optimize unified peer review, while Taechoyotin et al. [739] extend multi-agent scientific reviews to multimodal scenarios.

7.2.2. Meta-Review Generation

Meta-review generation synthesizes multiple reviewers' opinions into a single, objective, and comprehensive critique, emphasizing the manuscript's core contributions and limitations while balancing diverse viewpoints [395, 437, 298]. Early studies focus on guiding the summarization process through explicit structural cues [436, 663, 892]. More recent work addresses argumentative structures and latent biases among reviewers [114]. Notably, PeerArg [723] introduces a Multiparty Argumentation Framework (MPAF) that combines LLMs with knowledge representation to reduce subjectivity and bias. MetaWriter [728] automates the extraction of key arguments from reviewers. Darrin et al. [160] adapt the Rational Speech Act framework by creating a "distinctiveness score" to identify shared and unique perspectives across reviews. Moreover, Kumar et al. [397] introduce the ContraSciView corpus, which automatically detects contradictions between review pairs. Together, these efforts pave the way for more transparent and equitable meta-reviews.

7.3. Post-Review

Post-Review refers to the suite of AI-driven methods applied after a paper has passed peer review, aiming both to assess its future scholarly impact and to broaden its dissemination. It encompasses (1) influence analysis, predicting citation trajectories and research significance from the paper's content; and (2) promotion enhancement, automatically generating posters, lay summaries, videos, and other outreach materials to maximize visibility.

7.3.1. Influence Analysis

Influence analysis seeks to predict the future scholarly impact of a paper, most commonly measured by citation count, by evaluating its intrinsic characteristics [697, 327]. Early approaches predominantly rely on external metadata or handcrafted features, such as author reputation and journal impact factor [174, 740, 954]. In contrast, recent methods leveraging LLMs offer the advantage of directly inferring a work's innovativeness from its narrative. For instance, Zhao et al. [926] frame influence prediction as a regression task, fine-tuning an LLM on titles and abstracts to generate a time- and field-normalized impact score, effectively addressing the cold-start problem. Similarly, the HLM-Cite framework [277] adopts a two-stage approach: first, an embedding model retrieves a set of candidate citations from a large corpus, followed by a generative LLM

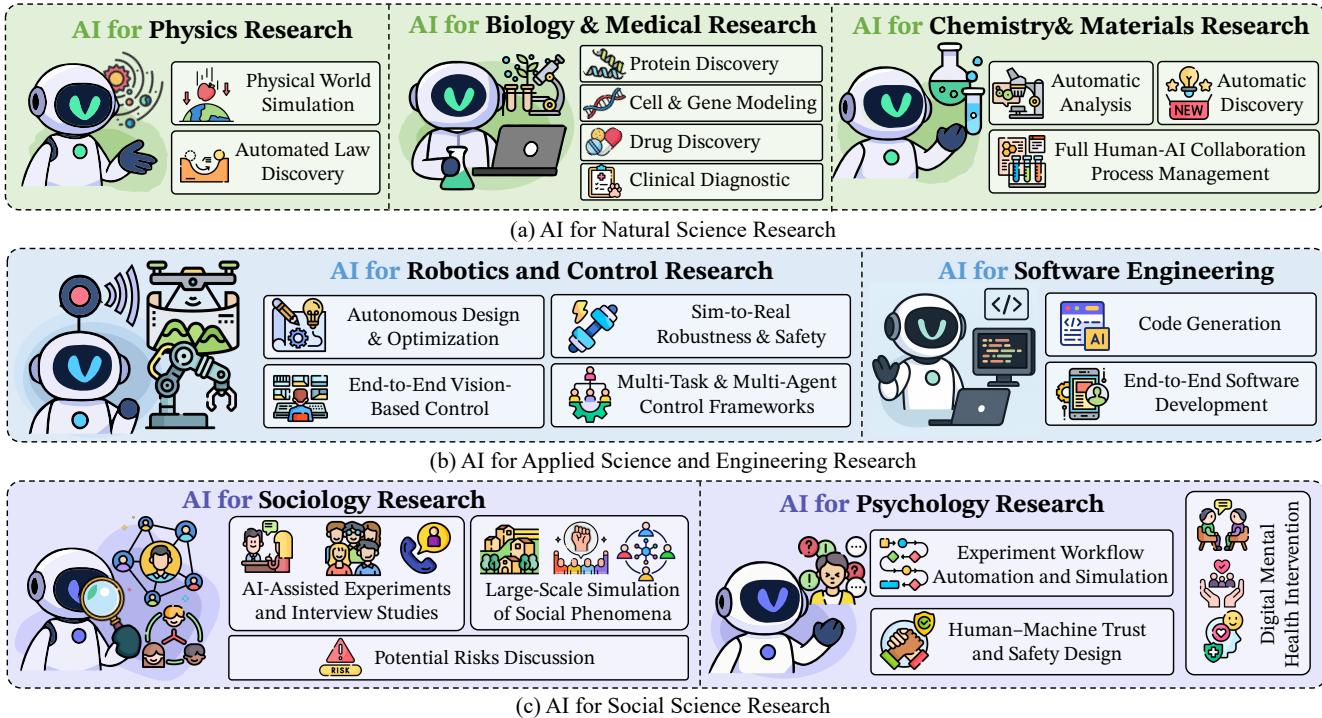


Figure 8: Multidisciplinary Applications of AI in Research. This includes three primary areas: (a) AI in Natural Sciences, covering fields such as physics, biology and medicine, and chemistry and materials science; (b) AI in Applied Sciences and Engineering, focusing on robotics and software engineering; and (c) AI in Social Sciences, encompassing disciplines such as sociology and psychology.

that performs fine-grained reasoning and re-ranking to identify the most relevant references.

7.3.2. Promotion Enhancement

Beyond predicting impact, a parallel research strand employs generative AI to amplify a paper’s influence by producing varied, accessible promotional materials. These tools convert dense scientific manuscripts into more inviting formats, thereby broadening their reach. For instance, Sun et al. [731] present the P2P system, which automatically generates academic posters from lengthy, multimodal documents through intelligent content selection and optimized layout design. To improve public understanding, Markowitz [534] leverage GPT-4 to produce lay summaries and demonstrate that these AI-generated summaries surpass human-written ones in linguistic simplicity. More recently, Park et al. [593] introduce SciTalk, a multi-agent framework that generates concise scientific videos. The rapid proliferation of such systems highlights the critical need for robust evaluation, leading to the creation of specialized metrics for assessing the quality of AI-produced scientific communications [297].

8. Application of AI for Research

As shown in Figure 8, it contains three main categories: AI for Natural Science Research (§ 8.1), AI for Applied Science and Engineering Research (§ 8.2) and AI for Social Science Research (§ 8.3).

8.1. AI for Natural Science Research

8.1.1. AI for Physics Research

In physics research, AI is now indispensable for developing new methodologies and driving discoveries [177, 67]. Its applications range from automated law discovery to physical world simulation and neural operator learning, all aimed at improving simulation accuracy, speeding up computation, and revealing hidden patterns from limited data [348, 811, 544].

Physical World Simulation integrates physical priors with AI models to simulate complex systems while enforcing consistency with physical laws [47, 164, 632]. Earlier, Physics-Informed Neural Networks (PINNs) [631] embed PDE constraints in the loss function, allowing them to solve and infer nonlinear equations from sparse data. By exploiting the conserved-quantity structure of Hamiltonian mechanics, Hamiltonian Neural Networks [254] exploit conserved-quantity structures to enforce energy conservation, yielding faster convergence and drift-free, reversible simulations. Lagrangian Neural Networks [151] parameterize the system's Lagrangian directly, avoiding coordinate choices, while still preserving exact energy conservation in examples like the double pendulum.

Automated Law Discovery leverages the reasoning power of LLMs, automated law discovery systems generate, test, and refine physical laws from noisy experimental data [684, 686]. For instance, AI-Newton [196] autonomously derives and validates physical laws, such as Newton's laws and conservation principles, without requiring operator-provided equations. By integrating a solid knowledge base with a structured discovery workflow, AI-Newton generates interpretable models of physical phenomena. Shojaee et al. [684] propose a novel method utilizing LLMs' scientific knowledge and code-generation capabilities to discover scientific equations directly from data. The DrSR framework [798] enhances law discovery by analyzing structural data relationships and implementing a feedback mechanism, improving performance across various domains. LLM-Feynman [709] combines automated feature engineering, LLM-based symbolic regression, and formula interpretation to extract interpretable expressions from both empirical data and domain knowledge. Recently, Li et al. [441] use enhanced visual prompting with domain expertise to uncover physical coordinates and governing equations from high-dimensional datasets more efficiently.

8.1.2. AI for Biology & Medical Research

Artificial intelligence in the life sciences and medical research uses algorithms and computational models to analyze and predict across scales [408, 446, 861, 784, 80], from molecular structures to clinical diagnostics [828, 150, 801], to accelerate drug discovery [744, 581, 261], optimize experimental workflows [735, 330, 565], improve diagnostic accuracy, and advance precision medicine [346, 366, 860, 318].

Protein Discovery. A notable example of computational innovation is Protein Discovery and protein structure prediction, which aims to predict the three-dimensional atomic structure of proteins. This is key for understanding biological functions and guiding drug design [173, 233, 235, 594]. For instance, Senior et al. [671] show that deep learning-based distance predictions significantly enhance de novo folding accuracy. The AlphaFold 2 system, developed by Jumper et al. [355], achieves atomic-level precision and has transformed structural biology since 2021. AlphaFold 3 [2] builds on this by introducing a diffusion-model architecture that predicts monomeric structures and reconstructs protein-nucleic acid and protein-ligand complexes with near-experimental accuracy. Additionally, Lin et al. [475] present a dual-task LLaMA-based framework that integrates reaction and retrosynthesis into a unified recombination-fragmentation process, generating novel compounds with strong predicted protein-binding affinities through molecular docking feedback.

Cell & Gene Modeling. A crucial area of research is cell-level modeling and gene expression analysis, aiming to simulate cellular behavior and identify activity changes under various conditions [81, 226, 650]. Several studies focus on pretraining models to improve cell or gene modeling [124, 61, 148]. However, due to the scarcity of high-quality gene and cellular data, recent work has explored data augmentation techniques to enhance AI training data [6, 530, 11]. Additionally, Roohani et al. [651] introduce an agent-based intelligent system that designs novel experiments, reasons about outcomes, and efficiently navigates hypothesis space by utilizing external tools to search the biomedical literature, analyze datasets, and engage secondary agents for evaluation, thus converging on optimal solutions. Furthermore, recent research has investigated AI-driven autonomous medical procedures, positioning AI as a collaborative tool for researchers [959, 845]. The micro-STAR system [284] integrates real-time OCT imaging with AI tissue classification to autonomously perform vascular suturing on ex vivo vessels, achieving leak-pressure performance comparable to expert surgeons, thus demonstrating the potential of AI and robotics in minimally invasive surgery.

Drug Discovery In recent years, artificial intelligence (AI) has made significant advancements in the field of drug discovery, driving multi-faceted innovations in drug design and showcasing immense potential and prospects [269, 744, 186]. **(1) Structural Prediction and Molecular Design:** AI has made notable progress in structural prediction and molecular design. Early studies [718] use deep learning models to screen 23 potential antibiotic candidates from over 107 million molecules, successfully identifying a drug with antimicrobial activity. The LUMI-lab platform [153], which integrates molecular models with automated experimentation, discovering ionized lipids that excel in mRNA delivery. However, challenges related to data scarcity persist in AI-driven drug discovery. To mitigate this, strategies such as multi-target drug polypharmacology, decoding drug responses, and quantum computing have been proposed to enhance model performance [222]. **(2) Multi-Agent Collaborative Drug Identification:** Multi-agent systems have proven highly effective in drug discovery, facilitating the rapid identification of new therapeutic compounds [419]. For instance, the DrugAgent [495] and DrugPilot [432] automate machine learning programming through multi-agent collaboration, achieving full automation from data acquisition to model evaluation, thus improving efficiency. Solovev et al. [702] introduces multi-agent approach that combines LLMs with specialized generative models and validation tools to automate the end-to-end drug discovery process. Lee et al. [419] develop a multi-agent framework that retrieves and integrates information from biomedical knowledge bases to generate responses, avoiding the need for expensive domain-specific fine-tuning. Despite these advances, challenges remain in addressing data quality, model interpretability, and regulatory hurdles [581, 884]. **(3) Drug Repurposing:** Drug repurposing involves the use of approved drugs for new therapeutic indications [511, 317]. In liver fibrosis research, the AI-assisted Collaborative Scientist system has successfully recommended drugs with significant anti-fibrotic activity using human liver organoid platforms, showing promise for treating liver fibrosis [261]. By integrating knowledge graphs and diverse data sources, Liu et al. [495] and Gharizadeh et al. [237] identify potential drug repurposing candidates and provide interpretable predictions. Lee et al. [420] combine subgroup analysis and treatment effect estimation, simulating clinical trials to identify drug candidates and characterize patient subgroups based on treatment effects. This approach, tested on a real-world database of more than 8 million patients, simulate over 1,000 drug trials, identifying 14 drug candidates beneficial to specific subgroups.

Clinical Diagnosis Clinical diagnosis advances through three converging breakthroughs. **(1) Clinical Brains:** First, LLMs serve as clinical “brains”, matching physician-level performance on medical licensing examinations [77, 252, 374, 695, 828]. Further, to enhance transparency and structure in decision-making, a human-AI note-taking framework [150] and Long-CoT reasoning techniques [411] has been proposed, leveraging case-based reasoning to guide clinical inquiry. **(2) Multi-Agent Hospital Simulation:** Multi-agent systems such as Agent Hospital replicate AI-AI [195, 403] and human-AI [665] collaborative diagnostic and treatment workflows, effectively serving as an organizational “nervous system” for care coordination [431, 39].

(3) Interactive Physical Actuation: Robotic platforms guided by LLMs perform precise physical interventions. For example, an autonomous optical coherence tomography system delivers surgeon-level accuracy in delicate procedures such as vascular anastomosis [284]. Together, these breakthroughs demonstrate the feasibility of fully autonomous medical facilities in which artificial agents seamlessly integrate diagnostic reasoning, therapeutic planning, and procedural execution.

8.1.3. AI for Chemistry & Materials Research

AI-driven automation in chemistry [285, 520, 554] and materials [613, 347, 136] integrates machine learning, robotics, and instrumentation into a closed-loop system for design, synthesis, and characterization, speeding decisions and experiments [116, 887, 832].

Automatic Analysis seeks to identify optimal or novel material compositions in virtual or automated experimental setups while minimizing the number of required experiments [46, 633, 672]. Specifically, Chen et al. [102] introduce MEGNet, demonstrating that graph neural networks can achieve density functional theory-level accuracy for both molecular and crystalline properties. Li et al. [452] employ two-stage Bayesian optimization to screen 560 organic photocatalysts using only 2.4% of the experiment conditions, thereby obtaining significantly improved performance. Ekosso et al. [189] combine low-cost robotic platforms with high-throughput microscopy and Gaussian process models to map vesicle formation processes. More recently, Szymanski et al. [737] implement a robot-machine-learning platform that accelerate compound discovery and identify 41 novel inorganic materials within 17 days.

Automatic Discovery is an automated experimental platform that combines robotic operations, online characterization, and real-time decision-making algorithms to autonomously execute the full experimental process, from reagent dispensing to result analysis [83, 460, 161]. Early research laid both theoretical and practical foundations: Butler et al. [83] review machine learning methods that accelerate materials design and discovery [548, 158, 324]. Furthermore, Dai et al. [155] employ a mobile robot with UPLC-MS and NMR to plan and interpret syntheses in a manner akin to human chemists. Jayarathna et al. [339] leverage literature data to reduce the number of experiments in an active-learning loop, discovering new Ru-based catalysts. Dai et al. [156] introduce an AI advisor for ion-electron polymers, improving performance by 150% over spin-coating methods. More recently, several studies have incorporated LLMs to enhance innovation and knowledge in chemistry and materials discovery [910, 863, 390].

Full Human-AI Collaboration Process Management leverages LLMs or natural-language understanding and generation to support hypothesis formulation, experimental design, and iterative optimization, aiming to facilitate more intuitive and efficient research interactions [785, 515, 424]. The AILA framework [531] embeds LLMs within a fully automated atomic-force microscopy workflow, illustrating both the potential and current constraints of language models in guiding real-time microscopic experiments. Sprueill et al. [711] and Feng et al. [206] integrate LLM-driven linguistic reasoning with chemical feedback in a heuristic search loop to propose novel catalysts and reaction pathways within uncertain chemical spaces. Recognizing that collective intelligence often outperforms individual reasoning, several studies [568, 707, 406] employ multi-agent architectures in which LLMs generate hypotheses, design experiments and direct iterative optimization, thereby achieving seamless human-AI collaboration. Ma et al. [522] introduce the first fully automated retrosynthetic planning agent tailored for LLM-driven macromolecular design, enabling comprehensive enumeration of viable multi-branch reaction routes. Meanwhile, Zhu et al. [952] demonstrate a robotic AI chemist that performs ore pretreatment and catalyst optimization on Martian meteorite samples.

8.2. AI for Applied Science and Engineering Research

8.2.1. AI for Robotics and Control Research

AI for Robotics and Control Research applies AI methods: deep learning, reinforcement learning, and large language models, to the perception, decision-making, and control of robots, aiming to boost adaptability, robustness, and autonomy in novel environments [421, 413].

Autonomous Design & Optimization systems integrate robotics, machine learning, and domain expertise to automate experiment planning, execution, and optimization [460]. Uddin et al. [766] introduce OptoMate, a system using a fine-tuned language model for optical setup design and a robotic arm to assemble spectroscopy components with submillimeter precision, enabling cloud-based optical labs. Mieszczański et al. [551] employ computer vision and feedforward neural networks in a feedback optimizer to adjust 3D printing parameters in real-time, reducing data collection from days to hours and ensuring consistent part quality. Angello et al. [22] apply physically informed feature selection and supervised learning in a closed-loop system to enhance photostability and uncover solvent-mediated triplet-state mechanisms. Bu et al. [78] combine a text-conditioned video diffusion model with a feedback-driven controller to generate visual plans and iteratively refine actions, significantly improving performance.

End-to-End Vision-Based Control End-to-end vision-based control feeds raw images or video frames directly into a neural network to generate control signals, removing separate perception, planning, and control modules. Early work combine convolutional neural networks (CNNs) with reinforcement learning or guided policy search to map camera inputs to motion commands. Levine et al. [426] first apply Guided Policy Search to train perception and control jointly, mapping raw images to motor torques and demonstrating reliable real-world grasping. Levine et al. [427] train a CNN on massive real grasp attempts to predict grasp success in real time, closing the loop on novel objects. Kalashnikov et al. [358] introduce a self-supervised, closed-loop Q-learning framework trained on 580,000 grasps, enabling dynamic strategy adjustment, retries, and disturbance resilience. Tobin et al. [758] propose domain randomization, varying simulator rendering parameters so models trained on synthetic data transfer directly to real-world detection and grasping.

Sim-to-Real Robustness & Safety ensures reliable transfer of simulation-trained policies to real-world tasks while adhering to safety constraints. Bochem et al. [66] integrate sharpness-aware optimization into gradient-based RL to identify flat minima, enhancing transfer robustness in contact-rich tasks without compromising sample efficiency. Ayabe et al. [34] assess offline RL methods on a legged robot subjected to random and adversarial torque disturbances, revealing vulnerability to sudden perturbations and emphasizing the need for real-time adaptation and safety measures. Radosavovic et al. [627] train a Transformer-based controller using deep RL and deploy it outdoors for one week without safety scaffolding, showcasing adaptive performance amidst disturbances, rugged terrain, and varying payloads. Yang et al. [858] apply domain randomization for vision-based servoing of soft robots, eliminating the need for on-robot fine-tuning and enabling direct transfer of simulation-trained models to continuum manipulators. Guerrier et al. [263] combine control barrier functions with RL to enforce safety constraints during learning, preventing hazardous states in complex environments.

Multi-Task & Multi-Agent Control Frameworks facilitate concurrent task execution or enable collaboration among agents in complex workflows, thereby enhancing parallelism and automation. Tahmid and Notomista [741] introduce a reinforcement learning-based framework designed to dynamically learn and compose task policies in robotic systems with redundant architectures, incorporating time-varying priority stacks to adjust task priorities. Team et al. [752] propose a unified multi-agent system capable of automatically generating hypotheses, designing and conducting experiments, and refining methods through iterative feedback, establishing a closed-loop process that accelerates interdisciplinary research.

8.2.2. AI for Software Engineering

AI for Software Engineering Research focuses on applying AI techniques to automate software development tasks, enhance code quality, and improve developer productivity. This includes code generation, bug detection, code review, and software testing.

Code Generation refers to the use of AI models to automatically generate code snippets or entire programs from natural language descriptions or existing code patterns [657, 264, 438, 315]. This can accelerate the development process and reduce manual coding [508, 920]. For instance, Chen et al. [106] develop Codex, a GPT model fine-tuned on GitHub's publicly available code, which supports GitHub Copilot. To democratize program synthesis, Nijkamp et al. [571] train and release CodeGen, an LLM based on both natural and programming language data, alongside the open-source training library JAXFORMER. Additionally, several studies have explored advanced code capabilities and support for multiple programming languages, like Python, Java, and R [657, 264, 438].

End-to-End Software Development covers the entire software development lifecycle, with AI automating various stages [584, 193, 349, 415]. For example, Phan et al. [599] develop HyperAgent, a generalist multi-agent system designed to handle various SE tasks across different programming languages, mimicking human developers' workflows. Qian et al. [614] introduce Experiential Co-Learning, which enables software development agents to leverage historical experiences to improve task performance. Meanwhile, Qian et al. [615] introduce ChatDev, a chat-based framework for software development, and Kang et al. [363] present an explainable automated debugging framework powered by LLM-driven scientific debugging.

8.3. AI for Social Science Research

AI has been widely utilized to automate the design, execution, and analysis of social science experiments, encompassing tasks from hypothesis generation to data collection, with minimal human intervention. In this context, we will focus on two key domains:

8.3.1. AI for Sociology Research

AI in sociology research refers to the use of machine learning, natural language processing, and multi-agent systems to simulate, analyze, and explore social phenomena [506, 843, 367]. Through AI, researchers can reconstruct macro-level patterns of collective behavior and gain deeper insights into micro-level cultural contexts and individual interactions, thereby revitalizing traditional sociological methods [458].

AI-Assisted Experimental and Interview Studies. Controlled experiments and simulated interviews are increasingly employed by scholars to test social science hypotheses and evaluate the effects of various social mechanisms and policy interventions. Manning et al. [532] propose a methodology that combines structural causal models with large language models to automatically generate and empirically validate social science hypotheses in contexts such as negotiations, bail hearings, job interviews, and auctions. This approach effectively bridges the gap between theory and practice by utilizing the model both as a scientific tool for hypothesis generation and as an experimental subject for validation. Liu and Yu [484] develop MimiTalk, an automated interview system, and conduct a comparative study of AI-led and human-led interviews with 20 participants on the Prolific platform. This study demonstrates the feasibility of AI-mediated interviews and highlights their potential in experimental settings.

Large-Scale Simulation of Social Phenomena. This approach leverages algorithmic tools to automate the collection and analysis of extensive textual, visual, and interaction data to simulate and examine the macro-level dynamics of community practices and value evolution [294, 713, 326]. Perez et al. [598] automate

the extraction and analysis of large-scale text and image datasets to map cultural practices, value systems, and trends in contemporary online communities [877, 677]. Zamudio et al. [890] propose a simulation framework for cultural evolution using multi-agent LLMs, enabling the manipulation of network structures, individual traits, and biases in information transmission to investigate factors driving cultural diffusion and change. Chen et al. [121] develop a GPT-based three-module framework, including information extraction, variant generation, and outcome prediction, that achieved high consistency in predicting outcomes across 319 economic field experiments, while also reflecting the impact of gender, race, and social norms on performance. Additionally, Bao et al. [38] reveal the underlying, often unspoken codes within societies.

Potential Risks Discussion. While LLMs demonstrate strong predictive capabilities in the natural sciences, their performance in the social sciences remains limited. Manning et al. [532] find that, although LLMs can predict the signs of estimated effects well when given a proposed structural causal model, they struggle to predict the magnitudes reliably. Additionally, Luke et al. [512] highlight that LLMs face challenges in handling treatment effect heterogeneity and exhibit systematic biases when predicting social science outcomes. As such, LLMs' predictive capabilities are still underdeveloped, particularly in forecasting novel empirical patterns that could inform future experimentation [423].

8.3.2. AI for Psychology Research

Research methodology focuses on the design, implementation, and validation of psychological experiments to ensure validity and reproducibility [760, 429, 899].

Experiment Workflow Automation and Simulation. Recent research has explored integrating AI into the management and data simulation of psychology experiments [622, 788, 64]. Zamudio et al. [890] introduce the RAISE pipeline, automating the generation and validation of visual stimuli. In five experiments, AI-generated images match researcher-designed stimuli in both validity and recognizability. Cingillioglu et al. [141] conduct a fully automated online RCT with 1,193 participants, where AI managed recruitment, random assignment, intervention delivery, and data collection, successfully replicating eight classical hypotheses with gold-standard rigor. Cui et al. [154], Strachan et al. [719], Suri et al. [733] use GPT-4 to simulate responses for 154 classical experiments, reproducing 76% of primary effects but yielding 71.6% unexpected significant outcomes, illustrating the promise of AI-assisted replication while emphasizing the need for cautious interpretation [125, 172, 245].

Human-AI Trust and Safety Design. Research on human-AI trust explores the development of trust during human-AI interactions and derives strategies for ensuring safety [617]. Li et al. [454] introduce a three-dimensional framework encompassing the trustor, trustee, and context, identifying key factors influencing trust and offering design recommendations for improving safety. Building on this, Chandra et al. [96], through interviews with 283 individuals who have mental health experiences, develop a taxonomy comprising 19 risky AI behaviors and 21 negative psychological impacts. From this, they propose a multi-path case-method framework and a set of safety guidelines aimed at mitigating these risks.

Psychological Interventions. Psychological interventions increasingly employ AI-driven chatbots to provide scalable and cost-effective psychological support [607]. Earlier, Hagendorff et al. [273], Dillon et al. [172], and Binz and Schulz [64] discuss whether and when LLMs can replace human participants in psychological research, reviewing early evidence and proposing a theoretical framework while highlighting methodological caveats. In a randomized controlled trial, Heinz et al. [289] find that the Therabot chatbot resulted in significant reductions in clinical-level symptoms compared to the control group. Similarly, Spytska [712] explore the use of the Friend chatbot for crisis support, demonstrating that its efficacy is comparable to traditional face-to-face therapy. These findings highlight the potential of generative AI to enhance accessibility

Tool	Description
SciSpace Copilot	AI-powered Literature Q&A, Annotations, Auto-Summarization, Chart Explanations
Elicit	AI-powered Literature Q&A, Auto-Summarization, Suggestions
Jenni AI / NoteGPT	AI-powered Note-Taking, Auto-Summarization
Scholarcy	AI-powered Auto-Summarization, Summarization Card, Analysis and Organization
PDFMathTranslate	AI-powered PDF Math-Augmented Translation

Table 6: Representative and established AI systems and assistant tools for advancing scientific comprehension.

and effectiveness in mental health services, particularly in settings with limited resources [166, 167]. Recent work further demonstrates that LLMs can match or exceed human performance in generating emotionally resonant narratives [824, 654] and even pass standard Turing tests [354], underscoring their broader psychological and communicative capabilities.

9. Resources

To further advance research in this field, we will provide an expanded and more comprehensive suite of relevant resources, including tools, benchmarks, and datasets spanning all stages.

9.1. AI for Scientific Comprehension

9.1.1. Textual Scientific Comprehension

To advance the evaluation of scientific question-answering systems, various benchmarks have been developed with increasing task complexity and domain specificity [653, 862, 204, 287]. Table 6 presents a comprehensive overview of typical, mature AI systems and associated tools for scientific comprehension.

Datasets like ScienceQA [662], LitQA [407], LitQA2 [699], SciQA [32], SciQAG-24D [774], and TriviaQA [393] support QA for scientific content. SciBench [803] broadens scientific reasoning across physics, chemistry, and mathematics. Further, SciInstruct [896] broadens reasoning across formal proofs with instruction-tuned data [816, 772]. Moreover, AutoPaperBench [379] and SciCUEval [880] are proposed for automatic paper or scientific content understanding evaluation.

Furthermore, datasets have expanded into broader domains, including biomedicine [71, 350, 391, 639, 587, 474, 923], academic chemistry [120, 597], materials science [516], physics [938] and other scientific fields [850]. TheoremQA [115] evaluates AI models' ability to apply theorems to solve challenging science problems. Multi-task and multi-modal assessment frameworks, such as M3CoT [109], SciFIBench [643], MMSCI [455], SPIQA [605], and MultimodalArxiv [433], further extend these evaluations. To address broader multimodal and multi-document challenges, M3SciQA [430], SceMQA [465] and SciDQA [694] have also been introduced.

Beyond static benchmarks, dynamic and interactive evaluation frameworks have emerged. SCITOOL-BENCH [524] target tool use in scientific reasoning across domains, while Kuhn et al. [393] propose a multi-round dialog framework to simulate user interactions, introducing metrics like adjusted accuracy. In terms of generation alignment, Yu et al. [875] design a system to evaluate the semantic fidelity between generated content and scientific texts, combining automated scores with human judgment.

Tool	Description
Google Scholar / Web of Science / Scopus / AMiner	Literature Search, Citation Tracking, Author Profiles, Citation Analysis
Semantic Scholar	AI-Assisted Academic Search Platform (Semantic Graph)
Research Rabbit / Connected Papers / Citation Gecko / Iris.ai	Visual graph of Works
Scite.ai	Shows Citation Context (Supporting/Contradicting/Neutral)
Consensus.app	Opinion-based Literature Search, Ideal for YES/NO Questions
ResearchGPT	AI-generated Knowledge Graphs and Paper Structures

Table 7: Representative AI systems and assistive technologies that have been widely adopted to enhance academic surveys.

9.1.2. Table & Chart Scientific Comprehension

In the domain of reasoning based on charts and tables, a number of benchmarks have emerged to evaluate the ability of LLMs in both structural and logical comprehension. Early works, such as ChartQA [537], CharXiv [817], ChartX [842], MISSQA [931], and NovaChart [303], focus on assessing LLMs' performance in answering questions related to charts, utilizing both synthetic and real-world data. On the other hand, benchmarks like SUC [721], TableBench [837], and ToRR [28] emphasize the evaluation of LLMs' structural understanding, rather than content comprehension, across various tasks such as form interpretation, numerical reasoning, and textual analysis.

9.2. AI for Academic Survey

In the task of generating academic surveys, several representative public corpora stand out due to their distinct characteristics in terms of scale, domain, and structure. Table 7 presents a comprehensive overview of typical, mature AI systems and associated tools for academic survey collection and generation.

To evaluate the capabilities of scholarly retrieval systems, several studies have focused on the scholarly deep research [820], such as AcademicBrowse [942]. To facilitate section-level generation of related works, several large-scale datasets have been introduced, such as Cochrane [773], MSLR 2022 [791], MS² [170], and OARelatedWork [175], OAG-Bench [898]. These datasets pair comprehensive “Related Work” sections with their corresponding full texts, providing valuable resources for this task. Moreover, systematic benchmarks for evaluating the quality of automatic scholarly survey generation have been developed. Examples include SciReviewGen [368], BigSurvey [493], SurveySum [208], SurveyBench [855], AutoSurvey [807], and SurveyX [464]. These benchmarks provide critical metrics for assessing the performance of automatic systems in generating academic surveys. For fine-grained manual annotation, SurveyEval [786] offers a hierarchical title tree that includes a vast number of reviews and citations. It is accompanied by hierarchical consistency and citation-chapter alignment metrics, which serve as essential tools for evaluating the distribution of synopsis generation and citation accuracy.

9.3. AI for Scientific Discovery

To facilitate scientific discovery, a variety of AI datasets and tools have been developed to assist researchers in different stages of the research process. These tools range from experiment design and management to full-automatic discovery, as shown in Table 8.

Idea Mining has seen the introduction of several key resources that significantly contribute to scientific discovery tasks [105]. Notably, LiveIdeaBench [658], ResearchBench [502], Genome-Bench [874], AIdeaBench2025 [623], the AP-FRI Corpus [398], HypoGen [577], CLIMATEDATABANK [497], CHIMERA [717]

Tool	Description
<i>Experiment Design</i>	
SnapGene	Molecular Cloning and DNA Visualization
Elicit	AI-driven Experiments Design
<i>Experiment Management</i>	
Notion / Asana / ClickUp / Atlassian Rovo	Project Management, Task Tracking, Collaboration
Trello / Wrike	Generate Content, Help Brainstorming, Conceive Product
GitMind	Mind Mapping and Brainstorming Tool for Project Planning
Forecast	Project Risk and Status Management
Tableau / Power BI	Interactive Dashboards and Reports
<i>Experiment Conduction</i>	
Copilot / Cursor / Tabnine / Qodo	AI-powered Code Completion, Generation, Review, Documentation
Gemini CLI	AI-powered Open Source Command Line Tool
Diffblue	AI-powered Unit Test Generation for Java Code
MLflow / Weights & Biases / TensorBoard	AI Experiment Tracking And Visualization
Papers with Code	Paper-Code Pairs for Easier Reproducibility
MONAI	AI-powered Medical Imaging Framework for Reproducibility
Taskade	Generate Code Snippets and Debugging to Facilitate Collaboration Among Developers
<i>Full-Automatic Discovery</i>	
ChatGPT / Claude / Gemini	Problem Solving, Code Assistance, Writing Polishing, Full-Lifecycle Management
ResearchGPT	AI-generated Knowledge Graphs and Paper Structures
AutoGPT / OpenDevin	Multi-step Research Automation
AgentLabs	Multi-Agent AI Platform for Research Automation
AI-Scientist / Zochi	AI-powered Research Assistant for Scientific Discovery

Table 8: Representative AI tools and their role in facilitating scientific discovery, with a particular focus on experiment conduction.

and OMATO-Chem [867] provide structured datasets for idea mining and hypothesis generation, enabling systematic training and evaluation of LLMs. Furthermore, OAG-Bench [898] offers a comprehensive, fine-grained benchmark for academic graph mining, spanning 10 tasks, 20 datasets, and over 70 baseline methods, all curated by human experts. This resource fosters systematic evaluation and encourages community-driven research. Additionally, SPARK [664] and the ICLR-NeurIPS Ideas Dataset [442] introduce curated datasets of idea-centered abstract-review pairs from OpenReview submissions, supporting supervised and reinforcement learning for research idea generation with multi-dimensional idea quality control, including novelty, feasibility, and effectiveness.

Novelty & Significant Assesment In the development of automated scientific research evaluation, the academic community has primarily focused on the dual criteria of “novelty and significance”, systematically exploring the ability of language models to assess the innovation within scientific research [743]. The SchNovel framework [469] and NoveltyDetection [499] are introduced to evaluate AI systems’ capacity to assess scholarly novelty across multiple scientific disciplines sampled from arXiv, aiming to facilitate the automated evaluation of research originality in scientific workflows. Building upon this, Gu et al. [257] introduce BLADE, a system that integrates 12 expert-labeled datasets with multiple automated scoring methods, enabling the model to explore diverse inference strategies in open, data-driven scientific analysis. HypoBench [486], Dasgupta et al. [163] and Lin et al. [473] are designed to evaluate LLMs and hypothesis generation methods across multiple aspects, including practical utility, generalizability, hypothesis, novelty [163] and rigor [473] discovery rate.

Theory Analysis requires the collection of scientific evidence, theoretical verification, and theorem proving. Specifically, FV-Generalization Benchmark [589], SCitance [17], and MissciPlus [243] are designed to complete scientific evidence collection. TheoremExplainBench [392], XClaimCheck [365], SciNews [91], ClaimReview2024+ [75], FactKG [378], TrendFact [908], and SciVer [776] provide datasets and benchmarks for scientific verification analysis. MiniF2F [935], FIMO [482], MUSTARDSAUCE [325] are used to fine-tune and evaluate LLMs on scientific theorem proving tasks. Furthermore, datasets and benchmarks have expanded into broader domains, including biomedicine [814].

Experiment Design In terms of experimental design, Tian et al. [757] propose evaluation frameworks for zero-shot and few-shot scenarios within virtual screening and lead compound optimization, establishing a comprehensive set of metrics tailored for AI-driven drug discovery. Concurrently, Feng et al. [202] leverage 1.6 million bioactivity measurements to train a universal model using pairwise meta-learning, which facilitates rapid adaptation and robust generalization to new biological systems. For biological protocol understanding and reasoning, BioProBench [503] is the first large-scale, multi-task benchmark. In order to provide valuable insights for the safe and effective deployment of LLMs in medical domains, Zhang et al. [904] develop LLMEval-Med, a real-world clinical benchmark for medical LLMs with physician validation.

Experiment Conduction To evaluate model performance in realistic research environments, MLAGent-Bench [322], Exp-Bench [385], MLRC-Bench [919], MLE-Bench [95], DS-Bench [352], ScienceBoard [730], ScienceArena [932], AutoReproduce [929], SciReplicate-Bench [844], DO Challenge [700], and MLR-Bench [103] assess AI agents' abilities to perform typical research tasks, such as optimizing CIFAR-10 classifiers and tuning BabyLM. In a similar vein, Hu et al. [309] develop InfiAgent-DABench, which is based on real-world CSV datasets and evaluates models' ability to interact with tools in end-to-end data analysis tasks. MLGym-Bench [561] is the first Gym environment for machine learning tasks, enabling research on reinforcement learning algorithms for training such agents. ResearchCodeBench [312] enables continuous understanding and advancement of LLM-driven innovation in research code generation. AutoBio [412] is designed to evaluate robotic automation in biology laboratory environments.

Experimental Analysis Experimental Analysis involves systematically testing hypotheses, evaluating models, or validating theoretical assumptions to draw meaningful conclusions. MicroVQA [82] is proposed to assess three reasoning capabilities vital in research workflows: expert image understanding, hypothesis generation, and experiment proposal.

Full Automatic Discovery In recent years, benchmark suites have been developed to assess AI-driven research agents. These suites offer standardized datasets, predefined tasks, and evaluation metrics, thereby facilitating systematic advances in algorithmic optimization. They encompass multi-domain scenarios spanning chemical synthesis, materials discovery, and biological experimentation [257, 266, 481]. Notable examples include ScienceAgentBench [127], BaisBench [513], Curie [384], which are designed to evaluate AI scientists' abilities to generate novel discoveries in different disciplines through data analysis and reasoning with external knowledge [700, 685, 364]. And DiscoveryWorld [338] evaluates end-to-end scientific discovery agents, while DiscoveryBench [529] challenges large language models with 264 real-world and 903 synthetic tasks across six domains, using structured protocols to measure multi-step, data-driven discovery and to elucidate both capabilities and failure modes.

9.4. AI for Academic Writing

The field of AI in academic writing is supported by a comprehensive array of meticulously curated datasets that address various aspects of the academic writing process. Detailed tools are summarized in Table 9,

Tool	Description
EndNote / Mendeley plugins	Reference Insertion and Auto-Formatting
Mathpix Snip / MathHandwriting	AI-powered Math Equation Recognition and LaTeX Conversion
AI for Grant Writing	AI-powered Grant Writing Assistance
Writefull / Trinka / Grammarly AI / Paperpal / Overleaf Copilot / Wordtune	AI-powered Scientific English Polishing Tools
SciSpace Copilot / Jenni AI	AI Writing Assistants for Editing and Suggestions
ChatGPT / Claude / Gemini	Writing Inspiration, Summarization, Editing
GPT-4o / Vizcom / Illustrae / OpenArt	AI-powered Figure Generation and Illustration Tools

Table 9: An overview of representative AI tools and their contributions to enhancing academic writing.

which provides an overview of representative AI systems and their contributions to enhancing academic writing.

9.4.1. Semi-Automatic Academic Writing

Recent advancements in semi-automatic academic writing have led to the development of several datasets designed to assist researchers in different stages of manuscript preparation, writing, and editing.

Assistance During Manuscript Preparation. In the early stages of manuscript preparation, recent datasets such as MoDeST [84] and LLM-Rubric [281] offer valuable tools for generating multi-domain scientific titles and assessing the scientific idea generation capabilities of LLMs.

Assistance During Manuscript Writing Several datasets, including FigGen [646], SridBench [97], Figuring out Figures [90], SciCapenter [302], and TikZero [55], support figure and formula generation, from text-to-figure creation to automated TikZ code generation. For citation management, datasets like CITEWORTH [827], CiteBART [92], and ScholarCopilot [813] enhance context-aware automatic citation generation [107]. Additionally, FutureGen [35] extracts future work statements from thousands of papers, using LLMs to identify and validate forward-looking scientific content.

Assistance After Manuscript Completion. Once a manuscript is completed, further enhancement can be achieved through grammar correction and expression optimization. To support this process, datasets from the Automated Writing Evaluation (AWE) system [787], and AAAR-1 [507] provide valuable resources. Additionally, the transformer-based Feedback Dataset [940] offers comprehensive support for multi-dimensional writing quality assessment [335, 199]. Moreover, datasets such as Wikipedia Revision Histories [73], which track real-world editing histories, play an important role in refining language and improving overall clarity. Pang et al. [592] introduce the first benchmark and metric suite for poster generation for visual quality, coherence-language fluency, and the ability to convey core paper content.

9.5. AI for Academic Peer Reviewing

Research on AI for Academic Peer Reviewing is grounded in diverse datasets, addressing tasks from AI text detection to review generation, quality assessment, and decision support [944, 197, 635, 139, 138, 715, 48]. To simulate realistic peer review interactions, datasets such as ReviewCritique [180], PeerRead [360], SPOT [703], NLPeer [183], ReviewMT [742], MOPRD [472], OpenReviewer [329], MASSW [909], COMPARE [693], PeerArg [723], Re² [897], ReviewEval [382], AAAR-1 [507], Papereval [323], ORB [736] and ORSUM [893] collect extensive paper and review data from leading conferences or journals, enabling the training and evaluation of LLMs in multi-turn, long-context, or role-based peer reviews [601]. Additionally, LLMart [463] offers a toolkit for evaluating LLM robustness through adversarial testing and prompt optimization, ensuring AI reliability in sensitive academic contexts. To assess LLM review quality more precisely, Shin

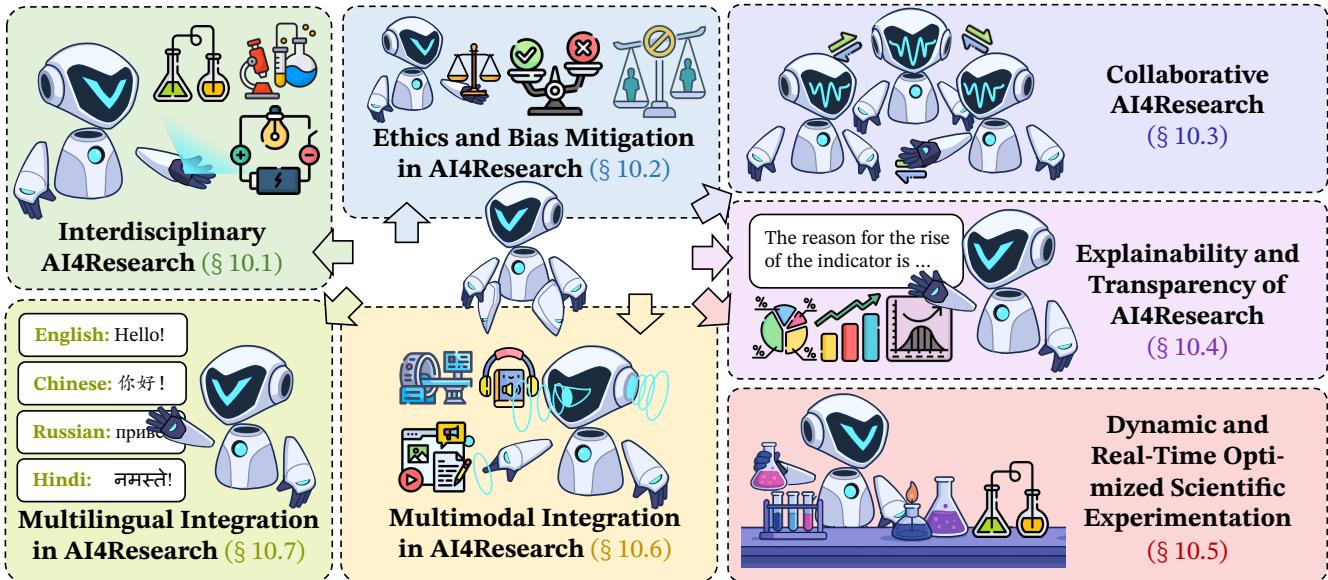


Figure 9: Frontiers and Future Directions of Artificial Intelligence in Research: This includes (1) Interdisciplinary AI models, (2) Ethics and Safety in AI4Research, (3) AI for Collaborative Research, (4) Explainability and Transparency of AI4Research, (5) Dynamic and Real-Time Optimized Scientific Experimentation, (6) Multimodal Integration in AI4Research, and (7) Multilingual Integration in AI4Research.

et al. [682] and Couto et al. [149] analyze the quality of peer review content across multiple predefined aspects, highlighting discrepancies between LLM and human review focus.

In the field of review quality detection, researchers have investigated diverse quality features [238]. Purkayastha et al. [611], and PolitePEER [60] assess AI systems' ability to identify instances of “lazy thinking” or politeness in peer reviews. Furthermore, both the AI-Peer-Review-Detection-Benchmark [882] and TRIED [492] include thousands of AI-generated peer reviews alongside human-authored reviews from the ICLR and NeurIPS conferences. These datasets provide standard corpora essential for evaluating methods designed to detect AI-generated peer reviews.

10. Frontiers & Future Direction

10.1. Interdisciplinary AI Models

As AI advances across research domains, we need models that integrate knowledge from multiple fields. Future work should develop general-purpose AI systems able to understand and generate insights in biology, physics, social sciences, and beyond. The primary research directions are: (1) **Foundation Models**. This paradigm has become the cornerstone of cross-domain AI. These models are pretrained self-supervised on vast unlabeled or weakly labeled datasets, then fine-tuned on new tasks with minimal data. They have driven performance gains in medical imaging, natural language processing, and robotics [314, 375]. (2) **Graph Models**. Graph methods naturally handle relational data by propagating information along nodes and edges. This enables cross-field knowledge flow, e.g., integrating ontologies and neural graphs in medical text classification for precise concept capture and efficient inference [192, 79, 260, 474, 410].

The greatest challenges at present are: (1) **Heterogeneous Interdisciplinary Data**. Interdisciplinary research involves diverse modalities, from high-dimensional sensor signals to categorical labels and unstruc-

tured text. These sources vary in scale, noise characteristics, and missing-data patterns, hindering unified preprocessing and feature fusion [612, 870, 143]. **(2) Cross-Domain Knowledge Transfer.** Transferring knowledge across domains requires extracting and adapting relevant information for new tasks. Techniques such as policy transfer, domain-adversarial training, and semantic alignment can narrow some gaps, but negative transfer persists in highly heterogeneous settings [574, 673]. Moreover, preserving reliability and interpretability during transfer, to ensure more applicable and trustworthy application in novel contexts, remains an urgent open problem [953].

10.2. Ethics and Safety in AI4Research

As AI assumes a central role in scientific research, a range of ethical, safety, fairness, and bias concerns has emerged [209, 871, 241, 319], making mitigation essential [18, 249, 848, 590, 132]. Early work by Farber [197] shows that, while AI improves reviewer matching and response rates, it disadvantages authors in low-resource languages or on niche topics. Worse, text-similarity matching can be abused by collusive rings to manipulate peer review, underscoring the need for built-in anti-collusion measures [629, 300]. Moreover, McShane et al. [541] find that AI-assisted statistical interpreters fall prey to “dichotomous mania”, reducing results to simply significant or not, a flaw that prompt-engineering alone has not resolved [637]. There are two main mitigation strategies: **(1) Fairness-Aware Training:** Integrate fairness constraints into the loss function to balance accuracy and equity across groups [209, 276]. Causal-inference methods then detect and adjust for hidden biases, enabling counterfactual fairness interventions [130, 547]. **(2) Training-free Debiasing:** Without retraining, apply unsupervised pruning and reweighting to model outputs at regular intervals, correcting biases in large language models by leveraging their pretrained behaviors [184, 652, 131]. **(3) Establishing Ethical Framework:** Some studies are establishing benchmarks for professional and broad ethical frameworks to regulate AI-generated content in a controlled area through security risk and ethical issue monitoring [949, 710].

Nonetheless, these endeavors confront two core challenges: **(1) Balancing performance and fairness:** The inherent tension between maximizing predictive accuracy and enforcing fairness constraints is difficult to reconcile and typically demands meticulous, application-specific tuning to avoid degrading model utility [291, 726]. **(2) Avoiding AI Plagiarism:** A major ethical concern in AI-driven scientific research is plagiarism [477, 220, 826]. Large-scale text generation by LLMs could lead to a “plagiarism singularity”, where text originality is diminished, raising concerns about the ethical and copyright risks of AI-generated content [634]. Studies have also revealed significant instances of intelligent plagiarism in LLM-generated scientific literature [270].

10.3. AI for Collaborative Research

As interdisciplinary research advances, the diversity of team members’ backgrounds can impede information flow and decision coordination. AI techniques can automatically extract and synchronize cross-document and cross-domain information, thereby narrowing the information gap among collaborators [65, 667]. Simultaneously, AI-driven arbitrators within real-time collaboration platforms can adjust task allocation dynamically based on project progress and member expertise, improving both efficiency and the quality of innovative outcomes [509, 201, 299]. The main research directions can be broadly divided into two categories: **(1) Collaborative Agents and Cooperative Intelligent Systems.** Collaborative agents are AI systems endowed with decision-making, autonomous execution, and communication capabilities. They simulate and augment human collaborators by participating in complex project management and research workflows through task assignment and autonomous role switching [299, 306]. Through semantic retrieval, reasoning validation, and context awareness, multi-agent frameworks are creating a new paradigm of human-AI collective intelligence, enabling automated hypothesis generation, experimental design planning,

and preliminary results analysis to accelerate scientific discovery [958, 432, 713]. These advances support efficient human–AI hybrid teams and suggest fertile directions for further work on collaborative agents and distributed modeling. **(2) Federated Learning and Distributed Modeling Mechanisms.** Because sensitive data across institutions cannot be fully shared, recent research has adopted federated learning as a privacy-preserving distributed modeling approach. By training models collectively while keeping data local, federated learning mitigates data silos among institutions and specialist teams [434, 895, 400]. To enhance both performance and privacy guarantees, differential privacy, and homomorphic encryption are being integrated with federated optimization algorithms, offering scalability and regulatory compliance for large-scale, multi-scenario collaborative research [763].

Current challenges in this field include: **(1) Interaction Complexity.** Repeated task reassignments, control handovers, and heterogeneous communication modalities can lead to misunderstandings, inefficiencies, and compounded coordination errors [246, 296]. Addressing this issue requires adaptive collaboration mechanisms that allow AI systems to adjust their behavior dynamically to match human collaborators' working styles and decision-making preferences. Multi-intelligence relationships are also critical, with three failure modes of miscoordination, conflict, and collusion [274]. **(2) Tension between Data Privacy and Accessibility.** A fundamental tension exists between data privacy and accessibility: stringent anonymization or legal restrictions often reduce the quality and diversity of training data. Although anonymization techniques and compliance with regulations protect privacy, they can diminish data utility and hinder AI models from capturing representative features, thereby affecting the accuracy and credibility of interdisciplinary research [557]. Moreover, differences in data access permissions, network bandwidth, and legal frameworks across institutions can cause communication delays and inconsistent model updates during distributed training, undermining the efficiency and stability of federated learning [262].

10.4. Explainability and Transparency of AI4Research

As AI models increasingly drive scientific discovery, ensuring their trustworthiness, transparency and explainability is essential. Future work should strengthen model interpretability so that researchers can trace how conclusions and recommendations are generated, particularly in high-stakes scientific applications [214, 188, 802]. Efforts to improve explainability fall into two main categories: **(1) White-box Analysis:** This approach investigates the model's internal structure by linking specific network “circuits” to conceptual representations. It has attracted considerable interest from both the security and transparency communities [57, 924, 630]. **(2) Black-box Analysis:** More recent work focuses on interpreting models without direct access to internal parameters. By examining reasoning trajectories and aggregate behavior, black-box methods provide insights into a model's knowledge representation and enable more reliable control over its outputs [85, 282, 108, 110, 112].

Despite these advances, two principal challenges remain: **(1) Lack of Standardized Frameworks:** Explanation techniques and metrics vary widely across the AI4Research community. Such absence can produce conflicting results and undermine user confidence. **(2) Transparency–Performance Trade-off:** Highly capable black-box models often sacrifice interpretability, whereas intrinsically transparent models may lag in performance. This tension complicates scientific adoption and raises uncertainty about whether novel outputs represent genuine discoveries or the recombination of existing data [477].

10.5. AI for Dynamic and Real-Time Optimized Scientific Experimentation

Real-time AI models can automatically adjust experimental protocols in response to unforeseen variables or shifting conditions, while performing immediate data analysis to substantially enhance research efficiency and innovative potential. Two prominent research directions have emerged: **(1) Agentic Real-Time AI:** This

approach advances AI beyond passive data analysis, transforming it into an autonomous research optimizing agent endowed with reasoning, planning, and decision-making capabilities based on real-time experimental feedback. Such agents can systematically survey the literature, generate hypotheses, design experiments, and iteratively refine workflows based on experimental feedback [460, 169, 156]. **(2) Coordination in self-driving laboratories:** These systems integrate robotic platforms, analytical instruments, and AI models into closed-loop frameworks that manage every stage, from experimental planning and execution to data processing. They support applications such as compound screening and novel materials discovery based on real-time signals with minimal human intervention [759, 87, 505].

Despite these advances, two core challenges must be addressed before dynamic, real-time AI experiments become routine: **(1) Reliable integration of heterogeneous devices and AI systems:** Laboratory environments comprise diverse instruments and robotic platforms requiring precise, real-time control and feedback. Systems must ensure compatibility, robustness, and low latency to avoid deviations or downtime caused by integration failures or timing mismatches. **(2) Low-latency decision-making and dynamic optimization:** AI-driven experiments must continuously ingest multisensor and instrument data on the millisecond to second timescales, update model parameters in real-time, and adjust protocols dynamically to maintain workflow continuity and efficiency. Simultaneously, they must uphold robustness and safety to prevent interruptions or hazards due to network jitter or computational bottlenecks [304, 305].

10.6. Multimodal Integration in AI4Research

As scientific data become more diverse, encompassing text, figures, tables, code snippets, and experimental signals, effective multimodal integration has emerged as a lynchpin for AI-driven discovery [109, 789, 795, 647, 135]. Early work [248, 122, 536, 678] show that jointly embedding text and figures can substantially boost deep analysis and literature-based discovery, yet this approach often falters when aligning highly specialized diagrams with their textual descriptions [134, 618]. There are two main integration strategies: **(1) Rigorous Multi-Source Data Ingestion:** Scientific datasets span manuscripts, high-resolution images, time-series signals, code artifacts, and structured tables. Each modality requires tailored preprocessing, such as OCR for figures, noise filtering for sensor data, syntax checking for code, to preserve integrity and alignment with domain ontologies [244, 425]. **(2) Interactive Human-in-the-Loop Refinement:** Unlike general-purpose systems, research workflows integrate expert feedback at multiple stages. Interactive interfaces enable domain scientists to validate figure captions, correct table alignments, or adjust the experimental setting based on the multi-modal signals, creating an iterative loop that refines model outputs and builds trust [691, 808, 925].

Nonetheless, multimodal integration in AI4Research faces two core challenges: **(1) Scarcity of cross-modal data and annotation bottleneck:** High-quality aligned annotations are exceedingly scarce, particularly in specialized scientific domains where expert involvement is required for fine-grained pairing, leading to a dramatic escalation of training and evaluation costs. **(2) Quantification of inter-modal uncertainty:** Data originating from diverse sources contain heterogeneous noise; how to uniformly quantify and propagate this uncertainty to support reliable scientific decision-making remains an open challenge.

10.7. Multilingual Integration in AI4Research

Scientific research transcends linguistic and geographic borders. Global initiatives, such as COVID-19 containment and climate modeling, depend on integrating literature, datasets, and expert insights across diverse languages efficiently. If AI tools favor only English or other high-resource languages, research sharing suffers, reinforcing “information silos” and the “knowledge divide” [20, 19]. Most researchers’ native languages lie in the “long tail” of AI systems. Neglecting low-resource languages limits discoverability

and citation of high-quality studies and sidelines region-specific topics (e.g., tropical agriculture, minority health). Multilingual pre-training and data augmentation can generate accurate summaries, retrievals, and translations in low-resource languages, breaking down academic barriers [147, 275, 140, 620, 604]. There are two principal integration strategies: **(1) Alignment of Scientific Terminology:** Reproducibility demands consistent terms and semantic fidelity. Multilingual terminology alignment and contextual-fidelity techniques ensure accurate translation of experiments and publications, so researchers worldwide build on a common knowledge base [660, 934, 216]. **(2) Equilibrating Multilingual Performance:** Data imbalances between high- and low-resource languages hinder cross-lingual transfer. Equalizing performance across languages enhances zero-shot and few-shot capabilities in research applications [140, 620, 796, 915].

Nonetheless, multilingual integration in AI4Research faces two core challenges: **(1) Balancing Capacity and Coverage:** Under finite computational and parameter budgets, striking the right balance between supporting core research capabilities and maintaining broad multilingual performance is critical to prevent “language breadth” from sacrificing “research depth”. This requires fine-grained architectural pruning and resource allocation tailored to specific domains and language pairs. **(2) Analysis of Cross-Lingual Academic Rhetorical Fidelity:** Ensuring that conceptual meanings remain consistent across different languages, preserving the logical integrity of academic argumentation in translation, and addressing language-specific academic conventions constitute important directions for future research.

11. Related work

Recent years have seen increasing interest in AI-assisted or autonomous research across multiple research communities [43]. The empirical use of large language models (LLMs) in research workflows indicates that most researchers are incorporating these models into their processes [466]. Additionally, Yu and Jin [878] survey and predict the rise in AI4Science publications, suggesting strategies to empower AI researchers. Early survey [10, 640, 918, 762, 913] summarize how LLMs are transforming scientific discovery [187, 939, 255, 951]. Li et al. [445] focus more on the ideation developments for LLM-assisted ideation, while Kulkarni et al. [394] and Ren et al. [642] summarize the architectures and benchmarks for LLM-driven discovery methods. Chen et al. [113] propose the Science-of-Science framework, which surveys the AI4Science in multi-agent simulation perspective. Meanwhile, Huang et al. [320] describe the AI-driven scientific discovery process from the perspective of the hypothesis lifecycle [334]. In particular, Zhou et al. [945] and Luo et al. [519] develop a three-stage taxonomy to systematically review assistance role in each phase. Building on this framework, Alkan et al. [15] and Bazgir et al. [51] offer a comprehensive classification of LLM-based hypothesis generation methods. In response to the peer-review crisis, Kim et al. [376] focus more on the bidirectional feedback system with certified reviewers, while Bolanos et al. [69] and Zhuang et al. [956] review the rise of automated scientific paper reviews, which coexist with human oversight.

Although significant advancements have been made in AI4Research, much of the existing survey has focused primarily on scientific discovery and academic writing, often under the umbrella of AI4Science or the limited research stages. However, these discussions typically overlook the broader research lifecycle, including scientific comprehension, academic survey, and peer review. Additionally, they tend to neglect AI applications across these stages. This paper introduces the AI4Research framework and offers a systematic survey of key factors and recent developments driving AI-enabled research. Our goal is to provide the research community with streamlined access to essential resources and insights, thereby facilitating innovative breakthroughs.

12. Conclusion

In conclusion, rapid advancements in artificial intelligence, particularly large language models like OpenAI-01 and DeepSeek-R1, have demonstrated substantial potential in areas such as logical reasoning and experimental coding. These developments have sparked increasing interest in applying AI to scientific research. However, despite the growing potential of AI in this domain, there is a lack of comprehensive surveys that consolidate current knowledge, hindering further progress. This paper addresses this gap by providing a detailed survey and unified framework for AI4Research. Our contributions include a systematic taxonomy for classifying AI4Research tasks, identification of key research gaps and future directions, and a compilation of open-source resources to support the community. We believe this work will enhance our understanding of AI's role in research and serve as a catalyst for future advancements in the field.

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