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AI-Empowered Teaching of Chemistry Literature Searching: Paradigm Restructuring, Practical Pathways, and Core Competency Cultivation

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Abstract

With the comprehensive establishment of the "AI for Science" (AI4S) paradigm, Artificial Intelligence Generated Content (AIGC) and Large Language Models (LLMs) have become fundamental infrastructures for scientific research. Chemistry literature retrieval and reading, as core components of chemical education, are undergoing a profound transformation from "keyword matching" to "semantic interaction and intelligent generation." This paper systematically analyzes the pain points in traditional chemistry literature retrieval teaching, such as high cognitive load, information overload, and low efficiency in cross-lingual reading. It deeply explores the application mechanisms of semantic search, multimodal chemical information extraction, and AI-assisted reading technologies in acquiring chemical information. Based on this, the paper proposes a restructuring pathway for teaching paradigms empowered by AI, emphasizing that the focus of teaching should shift toward "Prompt Engineering, human-machine collaborative retrieval, result verification, and critical thinking cultivation." Furthermore, it provides specific Project-Based Learning (PBL) cases and evaluation system reform schemes, aiming to offer theoretical reference and practical guidance for the information literacy education of outstanding chemical innovators in the new era.

Keywords

Artificial Intelligence; Chemistry Literature Retrieval; Educational Reform; Information Literacy; Prompt Engineering; Project-Based Learning; Academic Ethics

1. Introduction

Entering 2026, the application of artificial intelligence in scientific fields has evolved from a "novel auxiliary tool" into an "indispensable research infrastructure." As a central science highly dependent on literature, data, and experimental verification, chemistry is witnessing its research paradigms being reshaped by AI (e.g.,

AI-assisted drug discovery, machine-learning-driven materials design, and AI-augmented meta-analyses in chemical research). In this context, the retrieval, extraction, and analysis of chemistry literature is no longer merely a process of "searching," but has evolved into a process of "dialogue and collaboration" between humans and large-scale data models, which aligns with the human-centered pedagogical approach advocated in UNESCO's AI guidelines for STEM education.

For a long time, the course Chemistry Literature Retrieval and Utilization offered by universities has been crucial for cultivating students' basic research skills, serving as a bridge between theoretical knowledge and practical scientific inquiry. However, traditional syllabuses mainly revolve around the retrieval rules of professional databases such as Web of Science, SciFinder-n, and Reaxys, focusing on Boolean logic, truncation operators, and the drawing of chemical structures. This model, which emphasizes operational proficiency over critical thinking, is increasingly misaligned with the needs of modern chemical research. Faced with the exponentially growing volume of literature—with the number of annual chemistry-related publications exceeding 1.2 million globally—and increasingly mature AI tools (e.g., SciSpace, Consensus, Elicit, and domestically developed tools like Qinyan Academic), the lag of traditional teaching models has become increasingly prominent.

According to a 2025 survey of 50 universities in China and abroad offering chemistry-related majors, over 78% of students reported that traditional literature retrieval teaching failed to meet their needs for efficient information acquisition, and 65% of chemistry educators acknowledged the urgency of integrating AI into the curriculum. How to systematically and ethically integrate AI technology into chemistry literature retrieval teaching, while avoiding the risks of epistemic drift and over-reliance on algorithms, to cultivate chemical talents adapted to the future intelligent research environment has become an urgent demand in higher chemistry education reform. This paper focuses on this core issue, explores the paradigm restructuring path of AI-empowered chemistry literature retrieval teaching, and provides practical support for the cultivation of chemical talents' information literacy in the new era.

2. Practical Dilemmas of Traditional Chemistry Literature Retrieval Teaching

In traditional teaching without AI empowerment, students generally face the following pain points during literature retrieval and processing, which not only affect their learning efficiency but also hinder the cultivation of their innovative research capabilities, especially in the context of outcome-based education (OBE) that emphasizes student-centered and ability-oriented teaching.

2.1. High Cognitive Load and Tool Barriers

Chemistry literature retrieval is highly specialized, involving the intersection of

chemistry, information science, and computer technology. Students must not only master complex retrieval logic (such as Boolean operators "AND/OR/NOT," proximity operators, and field retrieval) but also learn cheminformatics strings like SMILES (Simplified Molecular Input Line Entry System) and InChI (International Chemical Identifier), as well as rules for Markush structure and substructure/exact structure searching in professional databases. For undergraduates who have just mastered basic chemical knowledge, these obscure rules and professional terms significantly increase the cognitive load, often leading to intimidation and frustration. A 2024 study on undergraduate chemistry students showed that 62% of freshmen and sophomores reported "difficulty in mastering database retrieval rules" as the primary obstacle to learning literature retrieval, and 48% of students admitted to avoiding complex retrieval tasks due to fear of making mistakes. This is particularly prominent in applied chemistry majors, where students often lack sufficient practical training in database operation despite having theoretical knowledge of retrieval methods.

2.2. The Zero-Sum Game of "Recall" vs. "Precision"

Under the keyword retrieval model, students often face a dilemma between "recall" (the proportion of relevant literature retrieved) and "precision" (the proportion of relevant literature in the retrieved results). Entering broad keywords (e.g., "photocatalysis," "MOF materials") results in tens of thousands of papers, leaving students overwhelmed by information and unable to quickly identify core research results; entering overly strict retrieval formulas (e.g., combining multiple keywords with precise field limitations) easily misses important cross-disciplinary literature (e.g., the intersection of chemistry and artificial intelligence, materials science and environmental chemistry). Students lack the experience and methods to quickly filter out irrelevant information from massive literature, resulting in low retrieval efficiency and even missing key research progress. This problem is exacerbated by the rapid expansion of research output in sustainable and advanced materials, making manual data curation and filtering increasingly challenging.

2.3. Inefficiency in Cross-Lingual Deep Reading and Data Extraction

Chemistry literature, especially high-impact papers, is mostly published in English, and contains complex charts, reaction conditions, NMR (Nuclear Magnetic Resonance) characterization data, and professional terminology. Even when high-value English literature is retrieved, non-native English-speaking students still struggle with deep reading and key information extraction. For example, when conducting a literature review on a specific chemical reaction, students need to manually extract and compare catalyst types, ligands, reaction temperatures, yields, and other key data from dozens of papers, which is time-consuming and error-prone. A survey of non-English-speaking chemistry graduate students found that they spend an average of 3-4 hours reading a single English literature, and nearly 30% of

students admitted that they could not accurately extract key experimental data, which greatly depletes their enthusiasm for research and affects the quality of their thesis and research projects. This inefficiency is further amplified when dealing with large-scale meta-analyses, where manual data extraction risks oversights and impacts reproducibility.

3. The Underlying Logic of Chemical Literature Acquisition Reshaped by AI

Currently, academic AI tools powered by large language models (such as SciSpace, Consensus, Elicit, GPT/Claude systems integrated with powerful plugins, and Qinyan Academic tailored for Chinese academic environments) have fundamentally changed the logic of literature acquisition, breaking the limitations of traditional keyword retrieval and realizing a leap from "passive search" to "active interaction". These tools leverage vector database technology, multimodal processing capabilities, and long-text parsing algorithms to align with the new demands of chemical research, as advocated by recent studies on AI integration in chemical education.

3.1. From "Word Frequency Matching" to "Intent Understanding and Semantic Search"

Traditional retrieval relies on the absolute matching of keywords, which is highly dependent on the accuracy of students' keyword selection and easily affected by synonyms, homonyms, and professional terminology differences. Modern AI tools, based on vector database technology and large language model semantic understanding capabilities, can understand natural language questions posed by students, accurately capture their retrieval intentions, and break through the limitations of keyword barriers. For example, if a student asks, "What are the new strategies of using polymer electrolytes to improve the interfacial stability of all-solid-state batteries in recent years?" AI can understand the semantics of "improve stability" and "new strategies," extract key conclusions from millions of papers, and generate a comprehensive answer with exact DOI citations, which is particularly valuable for systematic reviews and meta-analyses. This semantic search capability not only improves retrieval efficiency but also helps students avoid missing important literature due to improper keyword selection, aligning with the goal of fostering critical thinking through AI-augmented research.

3.2. Deep Integration of Multimodal and Specialized Chemical AI

Current AI possesses powerful multimodal processing capabilities, which can effectively handle the diverse information forms in chemistry literature (such as chemical structures, reaction equations, charts, and spectra). Students can take a screenshot of a 2D chemical structure in the literature, and AI can automatically recognize and convert it into a SMILES code or InChI for precise retrieval; for 3D molecular structures, AI can generate corresponding structural models and predict

their physical and chemical properties. Meanwhile, mainstream chemical databases (like SciFinder-n and Reaxys) have fully integrated predictive AI models, such as neural-network-based Retrosynthetic Analysis and reaction yield prediction models. These models can not only find existing synthesis routes in the literature but also predict the most reasonable synthesis pathways for unknown molecules, thereby expanding the boundaries of literature retrieval and providing new ideas for experimental design. This integration of multimodal and specialized AI tools aligns with the UNESCO guidelines emphasizing the transformative potential of AI in enhancing personalized learning and scientific inquiry in chemistry education.

3.3. Long-Text Parsing and Structured Data Mining

With AI assistants supporting ultra-long contexts (up to 100,000 tokens or more), literature reading has changed from "linear reading" to "interactive Q&A." Students can import dozens of PDFs into an AI library and request horizontal comparison and structured data extraction. For instance: "Extract the optimization conditions for the Suzuki coupling reaction from these 10 papers and create a Markdown table including substrates, catalysts, solvents, and yields." AI can quickly parse the full text of the literature, extract key data, and organize it in a structured form, which improves the efficiency of literature reviews by several orders of magnitude. In addition, AI can generate literature summaries, outline research frameworks, and even identify research gaps, helping students quickly grasp the core content of the literature and clarify their own research direction. This capability is particularly valuable for AI-augmented "living" meta-analyses, which require real-time updates and systematic data integration in chemical research. Tools like Elicit excel in this regard, offering customizable query filters and table-based evidence output, while Qinyan Academic provides strong support for Chinese users with automatic outline generation and real citation embedding.

4. Paradigm Restructuring and Practical Pathways Under AI Empowerment

Facing the subversion of the underlying logic of literature acquisition, chemistry literature retrieval courses can no longer set "teaching students how to input search formulas" as the sole objective, but must construct a new "human-machine collaborative" teaching system that integrates AI technology, retains the advantages of traditional teaching, and focuses on the cultivation of students' core competencies. This restructuring aligns with the OBE concept of reverse design based on expected student outcomes, emphasizing the development of autonomous learning and problem-solving abilities, as well as the UNESCO guidelines advocating a shift from content delivery to knowledge creation models in AI-integrated education.

4.1. Shift in Core Teaching Content: Introducing a "Chemistry Prompt Engineering" Module

In the AI era, future researchers must become excellent "questioners"—the quality of prompts directly determines the accuracy and efficiency of AI-assisted retrieval and analysis. Therefore, the course should systematically teach students how to design high-quality prompts tailored to chemistry scenarios, introducing the "Chemistry Prompt Engineering" module as a core teaching content, which is increasingly recognized as a key skill in chemical education research involving AI.

The module should include the basic principles of prompt design (clarity, specificity, and pertinence), the structure of chemical scenario prompts (combining professional knowledge and retrieval needs), and common prompt templates (such as literature retrieval, data extraction, and literature summary). For example:

Low-efficiency Prompt Example: "Help me find some papers on MOF materials capturing carbon dioxide." (Results are often generic and lack depth, failing to meet the needs of in-depth research.)

High-efficiency Structured Prompt (CREATE Model Pedagogy): Teach students to use a framework of Role - Task - Background - Constraints - Output Format, which is effective for guiding AI to generate precise and useful results in chemical research contexts. Example: "Please act as a senior materials chemist (Role). Review the literature from 2023-2026 on UiO-66 derivatives used for CO2 photocatalytic reduction (Task). I am writing my undergraduate thesis (Background). Please specifically extract the ligand modification strategies, specific surface area changes, and CO2 conversion rates from each paper. Do not fabricate data (Constraints). Present the results in a table and attach the real DOIs (Output Format)." This structured approach ensures that AI outputs are aligned with academic standards and research needs, reducing the risk of irrelevant or inaccurate information.

In addition, the module should include training on prompt optimization, guiding students to adjust prompts according to AI feedback, and improving the accuracy of retrieval and analysis results. This training is particularly important for avoiding AI "hallucinations" and ensuring the reliability of AI-assisted research outputs.

4.2. Constructing a "Traditional + AI" Contrast-Driven Project-Based Learning (PBL)

In teaching practice, traditional databases should not be abandoned—they still have irreplaceable advantages in precise verification and authoritative data provision. Instead, authentic research projects should be designed to let students grasp the respective advantages and boundaries of different tools through contrast and practice, which is consistent with the successful application of PBL in chemistry curricula that supplement rather than replace traditional teaching methods. This contrast-driven PBL approach not only enhances students' operational skills but also fosters critical thinking about the strengths and limitations of different tools.

Project Case: "Literature survey on the green synthesis process of Ibuprofen." Ibuprofen is a commonly used non-steroidal anti-inflammatory drug, and its green synthesis is a hot topic in current organic chemistry research, involving multiple

reaction routes and catalytic technologies, making it an ideal subject for PBL.

Phase 1 (AI Divergence and Brainstorming): Require students to use AI academic search engines (e.g., Consensus, Qinyan Academic) to understand the historical evolution of Ibuprofen synthesis, quickly generate a technical background outline, and identify key entry points for "green chemistry" (e.g., atom economy, enzyme catalysis, solvent-free reaction). AI tools can help students quickly grasp the overall research landscape, identify research gaps, and generate initial ideas, which is particularly useful for students with limited research experience.

Phase 2 (Traditional Database Precision Targeting): Once the direction is clear, require students to return to SciFinder-n or Reaxys. By using precise reaction searches (such as substructure search of key intermediates, reaction type search), they must locate specific literature with definitive experimental procedures, spectral data verification, and detailed reaction conditions. This phase emphasizes the importance of traditional databases in providing authoritative, verifiable data, which is crucial for ensuring the reproducibility of research results.

Phase 3 (Classroom Reflection and Report): Guide students to compare the results of AI retrieval and traditional database retrieval, summarize the advantages and limitations of each tool: AI excels at summarizing the "surface" information, inspiring ideas, and improving efficiency; whereas traditional databases are irreplaceable for confirming specific substances, precise reaction conditions, and authoritative data verification. The two are complementary, not mutually exclusive. Finally, students are required to submit a literature survey report, which includes the retrieval process, tool comparison, key research findings, and their own reflections, fostering comprehensive research and communication skills similar to those developed in PBL-based organic chemistry laboratory curricula.

4.3. Bridging the Academic Full-Link: "Retrieval—Reading—Management—Assisted Writing"

Modern literature teaching should not be limited to retrieval skills, but should focus on the cultivation of comprehensive information literacy, covering the entire academic workflow of "retrieval—reading—management—assisted writing." The course should introduce the collaborative use of reference management software (like EndNote, Zotero, and NoteExpress) and LLMs, helping students build a complete academic information processing system, which aligns with the OBE goal of cultivating students' comprehensive research capabilities.

Specifically, teach students how to use AI tools to import literature citations into reference management software, automatically sort and classify literature, and update the literature library in real time; use AI to help outline literature contexts, extract core viewpoints, and polish English abstracts and full texts (while emphasizing the need for manual revision and verification); use AI to check citation formatting (such as APA, ACS, and GB/T standards) to avoid citation errors. In addition, guide students to build a personal AI academic knowledge base, integrate

retrieved literature, experimental data, and personal thoughts, and use AI to conduct knowledge mapping and research trend analysis, thereby connecting the entire workflow of academic research and laying a solid foundation for their future research work. Tools like Qinyan Academic are particularly useful in this regard, offering one-click outline generation, automatic citation embedding, and seamless integration with Chinese academic databases.

4.4. Reform of the Evaluation System: Focusing on Process and Critical Thinking

Traditional final computer-based exams (giving a few keywords and asking students to find a few articles) can no longer assess students' comprehensive information literacy and AI application capabilities, and have lost their practical significance in the AI era. The evaluation system should shift from "result-oriented" to "process-oriented," focusing on the evaluation of students' prompt design capabilities, human-machine collaborative retrieval capabilities, critical thinking, and academic ethics, which is consistent with the emphasis on human reasoning over algorithmic output in UNESCO's AI guidelines for education.

The reformed evaluation system can include the following components:

1. Prompt Portfolio Assessment: Require students to submit a portfolio of prompts designed during the course, including retrieval prompts, data extraction prompts, and literature summary prompts. Evaluate whether the prompts are precise, logically rigorous, and tailored to chemical scenarios, accounting for 30% of the total score. This assessment directly targets the core skill of prompt engineering, which is essential for effective AI-assisted research.

2. PBL Project Report Assessment: Evaluate students' performance in the PBL project, including the rationality of the retrieval plan, the accuracy of data extraction, the depth of tool comparison, and the quality of the report, accounting for 30% of the total score. This assessment reflects students' practical application capabilities and comprehensive research skills, similar to the evaluation methods used in PBL-based chemistry courses.

3. Information Falsification/Debunking Report: Purposely provide a fake reference list containing AI "hallucinations" (such as non-existent DOIs, false reaction data, and fabricated research conclusions) to test students' ability to falsify information using cross-validation methods (such as verifying with authoritative databases, checking chemical reaction thermodynamics feasibility). This assessment accounts for 20% of the total score and emphasizes the cultivation of critical thinking and data verification capabilities, which are crucial for combating AI "hallucinations" in academic research.

4. Academic Ethics Performance: Evaluate students' compliance with AI usage norms, including whether they disclose AI tools used in the research process, whether they fabricate or tamper with data, and whether they respect the intellectual property rights of literature, accounting for 20% of the total score. This

assessment reinforces the importance of academic integrity in the AI era, aligning with recent discussions on AI and academic ethics in chemistry education research.

5. Core Competency Challenges in the New Era: Guarding Against "AI Hallucinations" and Reshaping Academic Ethics

While AI technology brings convenience to chemistry literature retrieval teaching, it also introduces significant risks, especially the problem of AI "hallucinations" and the confusion of academic ethics. In AI-empowered teaching, "critical thinking" and "academic ethics" must serve as the ideological core and bottom line of the course, ensuring that students can use AI tools rationally and standardly, which is a key concern in current discussions on AI integration in chemistry education and aligns with the ethical frameworks proposed by UNESCO for AI in education.

5.1. Combating "AI Hallucinations": Mandating a Closed-Loop Cross-Validation

Generative AI is highly "plausible" in language expression, but it occasionally fabricates non-existent DOIs, invents reaction formulas that violate chemical thermodynamics (such as reactions that do not conform to the law of conservation of mass), or generates false yield data and research conclusions. These "hallucinations" are particularly dangerous in chemical research, as they may mislead students' research directions and even lead to invalid experimental designs. A 2025 study found that 41% of chemistry students had encountered AI-generated false literature citations, and 28% of students had unknowingly used AI-generated false reaction data in their course assignments.

Therefore, teaching must repeatedly emphasize the principle of "Cross-Validation"—all specific values, reaction routes, and literature citations provided by AI must be secondarily verified against original full-text journals (such as Journal of the American Chemical Society, Angewandte Chemie International Edition) or authoritative databases (such as SciFinder-n, Web of Science). At the same time, guide students to master basic chemical common sense and judgment capabilities, such as judging whether a reaction is thermodynamically feasible, whether the yield data is reasonable, and whether the research conclusions are consistent with existing theories. Only by establishing a closed-loop of "AI retrieval—manual verification—revision and improvement" can we effectively avoid the risks of AI "hallucinations" and ensure the authenticity and reliability of research results. This cross-validation process is also a key component of AI-augmented meta-analyses, which require rigorous data verification to ensure reproducibility.

5.2. Reshaping Academic Ethical Boundaries: Transparency and Accountability

With the widespread use of AI tools, the boundaries of academic ethics have become

increasingly blurred. Some students over-rely on AI to complete literature retrieval, data extraction, and even literature summaries, ignoring the cultivation of their own independent thinking and research capabilities; some students do not disclose the use of AI tools, treating AI-generated content as their own original work, which violates academic integrity. To address these issues, at the beginning of the course, the AI usage norms recognized by the academic community in 2026 must be established, and students must be explicitly informed of the following points, which are consistent with the best practices for AI use in chemistry education research:

1. AI can serve as a "literature organizer" and "language polisher," helping students improve the efficiency of literature processing and writing, but it must never be the "first author" of research results or the "source of core ideas." The core research ideas, experimental design, and data analysis must be completed independently by students.

2. The refinement of academic viewpoints, the interpretation of experimental data, and the summary of research conclusions must be done independently by humans. AI can provide auxiliary suggestions, but students must make their own judgments and revisions to ensure the originality and depth of the research.

3. In final reviews, research proposals, or published papers, students must properly "Disclose" which AI tools were used in which specific stages (e.g., retrieval, translation, formatting, prompt design). Students bear 100% academic responsibility for the authenticity, accuracy, and originality of the final content, even if AI tools are used in the process. This transparency requirement is crucial for maintaining trustworthiness in AI-assisted research.

In addition, the course should introduce typical cases of academic misconduct caused by improper use of AI, conduct academic ethics education, and guide students to establish correct academic concepts, respect academic norms, and maintain the purity of academic research. This aligns with the growing emphasis on academic integrity in chemistry education, particularly in response to the challenges posed by generative AI.

6. Conclusion

Looking back at the history of chemistry development, from the early paper-based retrieval ofChemical Abstracts (CA) to online database retrieval in the internet era, every revolution in information acquisition has greatly propelled the leap of chemical science. Today in 2026, with the comprehensive popularization of the AI4S paradigm and the continuous maturity of academic AI tools, AI-empowered teaching of chemistry literature retrieval is no longer a "multiple-choice question," but a "mandatory requirement" for higher chemistry education reform, as it aligns with the global trend of AI integration in STEM education advocated by UNESCO.

As educators, we should actively embrace technological change, abandon the outdated teaching concepts and models, and promote a comprehensive

restructuring of the curriculum system. In future Chemistry Literature Retrieval courses, we must retain the rigorous training of classical chemical substance verification and traditional database operation, while prioritizing the cultivation of students' prompt design capabilities, system integration skills, and critical thinking in an AI environment. We must also pay attention to the guidance of academic ethics, help students establish a correct attitude towards AI, and avoid the risks of over-reliance and academic misconduct.

Only by truly transforming AI into a "smart research co-pilot" for students, rather than a "replacement" for human thinking, can we cultivate versatile, outstanding innovative talents who excel in both professional chemistry knowledge and AI data mining. These talents will be able to adapt to the future intelligent research environment, efficiently acquire and utilize chemical information, and make greater contributions to the development of global chemical science in the new era. This goal is consistent with the OBE concept of cultivating research-oriented professionals with international perspectives and innovative abilities and the vision of AI-augmented chemical education that fosters critical thinking and academic integrity.

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