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AI Agent

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AI agents accelerate catalyst discovery for ultrafast water purification

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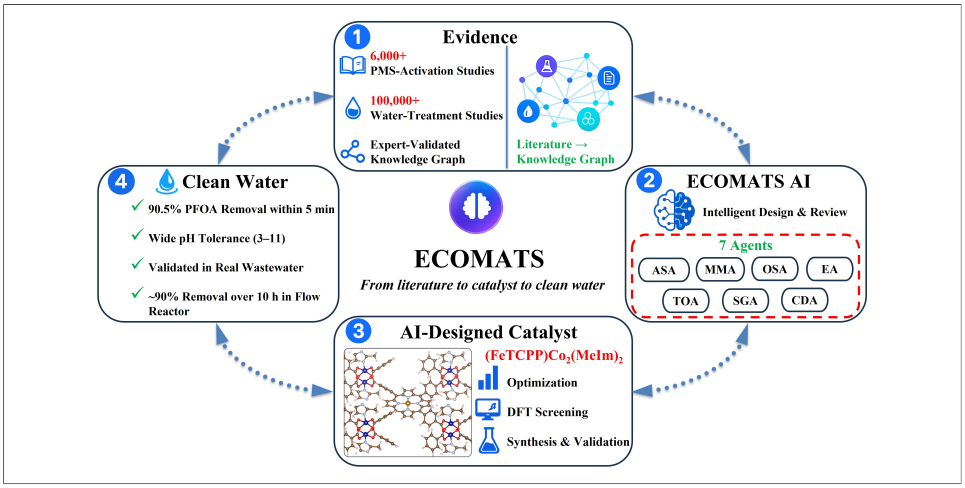

MAIN TEXT

Persistent contaminants such as perfluorooctanoic acid (PFOA) make water-treatment catalyst discovery a demanding materials problem[1]. In peroxymonosulfate (PMS)-based advanced oxidation, radical and non-radical pathways can both contribute to pollutant degradation[2], requiring catalysts to activate oxidants efficiently while remaining chemically plausible, synthetically accessible, and robust under realistic wastewater conditions. Conventional catalyst discovery, however, still relies largely on labor-intensive trial-and-error experimentation. Artificial intelligence (AI) agents can accelerate scientific discovery by coordinating specialized tasks, integrating diverse sources of knowledge, and supporting systematic decision-making across complex research workflows. Recently, Pan *et al.* developed ECOMATS, a seven-agent AI framework that integrates literature mining, candidate generation, mechanistic reasoning, multi-objective evaluation, operating-condition optimization and synthesis guidance into an AI-assisted catalyst-discovery workflow rather than an autonomous design platform[3]. This work reflects a broader transition

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from single large language models (LLMs) toward collaborative, tool-augmented AI agents capable of assisting multiple stages of scientific research rather than merely generating candidate materials[4,5].

A key contribution is the explicit positioning of AI as a research assistant that separates creative exploration from scientific validation. More than 6,000 PMS-activation studies were first converted into structured records and integrated with over 100,000 wastewater-treatment publications to construct an expert-validated knowledge graph. The framework comprises seven fine-tuned agents: one Task-Organizing Agent (TOA), one Creative-Designing Agent (CDA), three independent Assessment-and-Screening Agents (ASAs), one Mechanism-Mining Agent (MMA), and one Synthesis-Guiding Agent (SGA). The TOA decomposes and routes tasks, the CDA generates catalyst candidates, the three ASAs independently assess them, the MMA analyzes catalytic pathways, and the SGA proposes synthesis procedures. Candidate materials were subsequently evaluated across five complementary dimensions: catalytic performance (50%), economic viability (10%), environmental compatibility (10%), technical feasibility (10%) and structural validity (20%). Most importantly, a high-temperature design agent explored diverse chemical space, whereas three independent low-temperature assessment agents performed blind reviews whose scores were fused using a consistency-based weighting strategy [Figure 1A-C]. Each ASA produced a weighted total, and the three totals were fused using a consistency term that penalized inter-agent disagreement[3]. This multi-agent architecture fuses independent assessments while penalizing reviewer disagreement, providing more reliable screening than a single LLM. In benchmark testing, the fused score reached 90.7% classification accuracy against human-curated labels on a benchmark set of 100 candidates, comprising 70 high-quality catalysts, 20 low-quality controls, and 10 noise or structurally invalid candidates. Here, S_j denotes the final consistency-adjusted comprehensive score for candidate j on a 0-10 scale, integrating the weighted five-dimensional evaluation with cross-agent consistency. Candidates with $S_j \geq 7.0$ were selected for further evaluation[3]. This strategy highlights how AI can improve hypothesis prioritization while leaving scientific decision-making to human researchers. The AI-guided workflow ultimately prioritized five representative catalysts for PMS activation for human-led theoretical and experimental validation: (FeTCPP)Co_2(MeIm)$_2$, CoNi-BDC, AgV-MoS_2, FeCo-GrN and FeCo-g-C_3N_4. The highest-scoring candidate, (FeTCPP)Co_2(MeIm)$_2$, combines a porphyrinic Fe center with Co coordination through carboxylate and axial 2-methylimidazole ligands. Subsequent human-performed density functional theory (DFT) calculations showed that all five candidates possessed d-band centers within the favorable range for PMS activation and confirmed its designed coordination environment through X-ray photoemission spectroscopy (XPS) and X-ray absorption spectroscopy before evaluating its catalytic performance[3]. Experimental validation remained the cornerstone of the workflow. The optimized catalyst achieved 90.5% PFOA removal within 5 min, remained active across pH 3-11, and maintained approximately 90% removal efficiency during 10 h of continuous-flow operation [Figure 2A-C]. Successful gram-scale synthesis of the catalyst further highlighted the scalability of the AI-guided design strategy [Figure 2D]. Validation using wastewater samples collected from treatment plants across 31 provinces in China, with 84.3%-91.8% PFOA removal achieved within 5 min, further demonstrated the practical relevance of the AI-guided workflow under realistic water-treatment conditions rather than idealized laboratory environments[3].

The work should still be viewed as AI-assisted discovery rather than full automation. Despite the sophisticated multi-agent architecture, human researchers curated the literature input, carried out DFT calculations, synthesized the materials and verified performance. Moreover, the generated structures remained close to known catalyst families, reflecting the dependence of LLM-based systems on existing knowledge rather than exploration of entirely new chemical space. Data coverage, benchmark inconsistencies, and the absence of closed-loop experimental feedback also remain important constraints. Consequently, the framework primarily assists in prioritizing chemically reasonable hypotheses rather than autonomously discovering fundamentally new catalytic principles. Accordingly, AI primarily helps

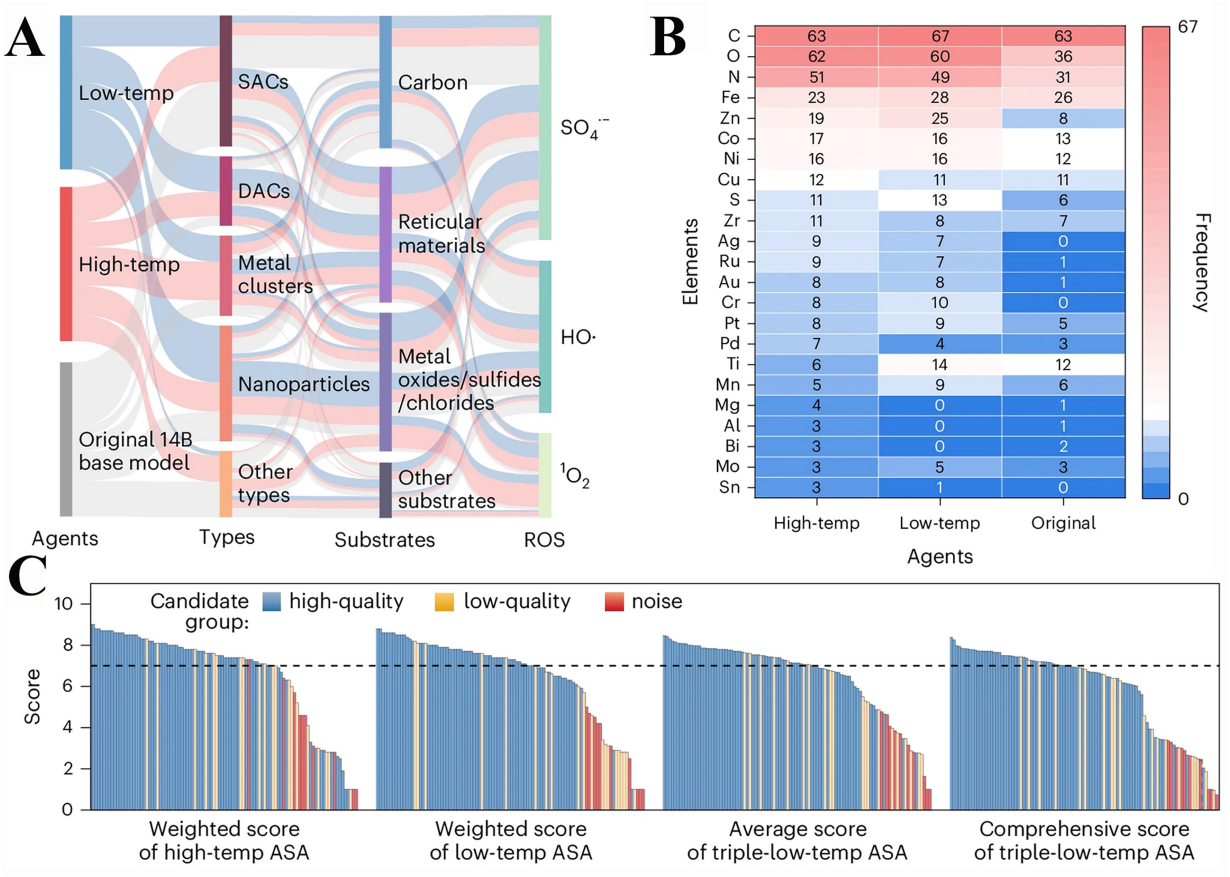

Figure 1. (A) Sankey plot of catalyst types, substrates, and dominant ROS generated by the high-temperature, low-temperature, and original Qwen3-14B model; (B) Heatmap of elemental frequencies in generated candidates; (C) Ranking of 100 literature-derived candidates by four scoring metrics. This figure is adapted with permission[3]. Copyright 2026, Springer Nature. ROS: Reactive oxygen species.

determine "where to search" and "what to test", whereas human researchers remain responsible for establishing the underlying physical and chemical rationale. Even so, ECOMATS offers a useful model for water-purification materials discovery: AI is most valuable when its proposals are constrained by chemical validity, mechanistic evidence, realistic operating conditions and tests in practical water matrices[6,7].

Future AI-assisted catalyst discovery should integrate mechanistic models, automated experimentation and active learning. Ultimately, frameworks such as ECOMATS may prove most valuable by positioning AI as a collaborative partner in mechanism-driven catalyst discovery.

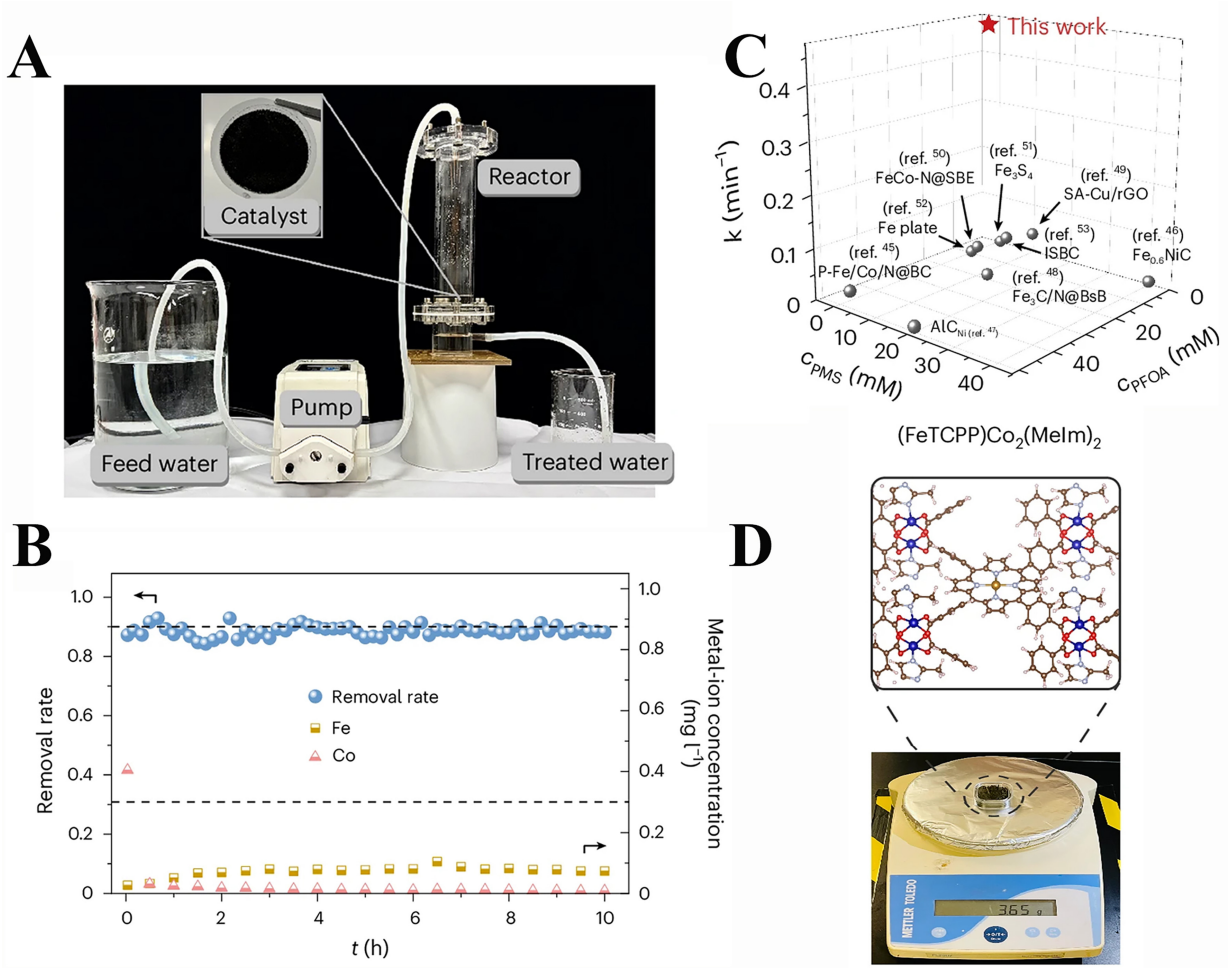

Figure 2. (A) Flow-through wastewater treatment setup; (B) PFOA removal efficiency and Fe/Co ion leaching using a membrane loaded with (FeTCPP)Co_2(MeIm)$_2$; (C) Comparison of the rate constant (k), PMS dosage, and initial PFOA concentration for (FeTCPP)Co_2(MeIm)$_2$ against reported PMS-activating catalysts; (D) Photograph of the gram-scale (FeTCPP)Co_2(MeIm)$_2$ sample with its structure inset. This figure is adapted with permission[3]. Copyright 2026, Springer Nature. PFOA: Perfluorooctanoic acid; PMS: peroxymonosulfate.

DECLARATIONS

Authors' contributions

Writing - original draft: Li, M.; Fu, Y.; Patial, S. K.

Writing - review & editing, supervision, funding acquisition: Fu, Y.; Ma, T.

Availability of data and materials

Not applicable.

AI and AI-assisted tools statement

Not applicable.

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Conflicts of interest

All authors declared that there are no conflicts of interest.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

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