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Review

Material intelligence by the convergence of artificial intelligence and robotic platforms

Xinyu Zhang,[1,2,12] Zijian Chen,[1,2,4,12] Feibei Chen,[1,3] Billy Fanady,[1] Boyuan Wang,[1] Zongming Ni,[1] Shumin Zhou,[1] Junzhi Ye,[11] Guanhua Chen,[7] Jie Liu,[7] Robert L.Z. Hoye,[11] Xiaobo Li,[6] Samantha Y. Chong,[10] Wei Feng,[2] Chi-yung Chung,[3] Ching-chuen Chan,[3] Linjiang Chen,[5,*] Han Hao,[9,*] Alán Aspuru-Guzik,[8,9] Jun Jiang,[5,*] and Haitao Zhao[1,3,*]

[1]PolyU-WIT Research Centre for Materials Intelligent Manufacturing, Wenzhou Institute of Technology (WIT), Wenzhou, China
[2]Center for Intelligent and Biomimetic Systems, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen, China
[3]Research Centre for Materials Intelligent Manufacturing, State Key Laboratory of Ultra-precision Machining Technology, Department of Electrical and Electronic Engineering, The Hong Kong Polytechnic University (PolyU), Hong Kong, China
[4]Department of Chemical and Environmental Engineering, the University of Nottingham Ningbo China, Ningbo, China
[5]Key Laboratory of Precision and Intelligent Chemistry, University of Science and Technology of China, Hefei, China
[6]Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Zhejiang Normal University, Jinhua, China
[7]Department of Chemistry, The University of Hong Kong, Hong Kong Quantum AI Lab, Hong Kong, China
[8]Department of Chemistry, Department of Computer Science, University of Toronto, Acceleration Consortium, Toronto, Ontario, Canada
[9]Department of Materials Science & Engineering, Department of Chemical Engineering & Applied Chemistry, University of Toronto, Vector Institute for Artificial Intelligence, Lebovic Fellow, Canadian Institute for Advanced Research (CIFAR), Toronto, Ontario, Canada
[10]Department of Chemistry and Materials Innovation Factory, University of Liverpool, Liverpool, UK
[11]Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK
[12]These authors contributed equally
*Correspondence: l.j.chen@bham.ac.uk (L.C.); hann.hao@utoronto.ca (H.H.); jiangj1@ustc.edu.cn (J.J.); hai-tao.zhao@polyu.edu.hk (H.Z.)
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BROADER CONTEXT

Traditional research in materials and chemistry relies heavily on trial-and-error material synthesis, labor-intensive testing, and human intuition in experiment planning. Recently, the rapid advancement of robotics and artificial intelligence has revolutionized a paradigm shift, enhancing both the precision and intelligence of materials science. In this review, we propose a comprehensive framework based on the interconnected cycles of "reading-doing-thinking," guiding rational design, enabling controllable synthesis, and facilitating inverse design, respectively. By embedding artificial intelligence into robotics, we introduce the concept of material intelligence, an approach that mimics and extends the way a scientist's mind and hands work and even beyond. Ultimately, by encoding material formulas and parameters into a "material code," we envision a universal material intelligence that can carry this code across time and space, enabling autonomous materials discovery all over the Earth and even on distant planets.

ABSTRACT

The emerging interdisciplinary research of material intelligence through the convergence of artificial intelligence, robotic platforms, and material informatics has revolutionized the field of chemistry and material science. This shift enables precision and intelligence in materials research to avoid the problems of trial-and-error synthesis and labor-intensive characterization. The aim of this review is to present a comprehensive methodology that unifies three interlinked domains: data-guided rational design ("reading"), automation-enabled controllable synthesis ("doing"), and autonomy-facilitated inverse design ("thinking"). We critically examine how the integration of materials common discipline (i.e., rational design, controllable synthesis, inverse design) with interdisciplinary research (i.e., data, automation, autonomy), with an emphasis on cutting-edge research of artificial intelligence and robotics, collectively shape a closed-loop next paradigm of material intelligence, revolutionizing experimental, theoretical, software-driven and data-driven paradigms. Ultimately, this paper discusses how these insights drive the new paradigm of materials research, which seamlessly combines database, robotics, artificial intelligence, and even embodied intelligence to empower the full potential of material intelligence.

INTRODUCTION

Advancements in artificial intelligence (AI) and robotics have profoundly transformed lab automation across diverse scientific disciplines, including pharmaceuticals,[1–3] biotechnology,[4] environmental testing,[5] and materials science.[6,7] In chemistry and materials science, this integration of AI and robotics, termed "material intelligence," enables unprecedented accuracy, efficiency, and adaptability in research and the commercial landscape.[8] Material intelligence is an interdisciplinary technology that focuses on enabling intelligent material synthesis through AI and robotics, similar to the way a scientist's mind and hands work and even beyond.

Material intelligence falls under the broad category of material informatics. While material informatics traditionally emphasizes computational modeling and database mining, material intelligence is more specific as it further integrates AI and robotic platforms to form a closed-loop experimental process. Such integration addresses a key limitation in material informatics, where reliability constraints are imposed by limited experimental data for high-quality data sources.[9] This shift transforms theoretical design into autonomous realization, enabling the real-time discovery and optimization of materials. For instance, while pioneering computational approaches like the Materials Genome Initiative, combinatorial synthesis, and inverse design methodologies have accelerated materials discovery,[10–12] they remain constrained by limitations in experimental validation and scalability. Material intelligence directly addresses these constraints, with automated robotic systems capable of precise, reproducible, and scalable synthesis, thereby reducing human error while enabling complex, high-throughput experiments. Additionally, changes are not limited to computational methods but also include experimentation, which leads to interdisciplinary research on data science in experimental chemistry,[13] automation[14] and the rise of self-driving labs.[15] Specifically, automation opens the door to new possibilities in enhancing the precision levels of materials synthesis processes through programmable robots and controllable synthesis parameters.[16] AI has further enhanced the intelligence of materials research, bridging the gap between informatics and experimentation by helping scientists generate hypotheses for rational design and obtain correlations for inverse design while continuously validating them through robotic experimentation.

As the integration between AI and automation continues to deepen, laboratory automation emerges as the practical enabler of these ambitions. Lab automation enables faster experimentation, reduces human error, and optimizes resource usage, leading to cost savings and quicker product introduction.[17] The successful transformation of the lab-automation landscape shows that automation systems are robust, accessible, and sustainable.[18] For instance, high-throughput screening in pharmaceuticals has cut down drug-discovery timelines by years, exemplifying how robust, accessible, and sustainable automation systems can transform the research and commercial landscape.[8] To sustain this momentum, the speed and efficiency of these methods must continue to evolve, aligning with the increasing complexity and demands of modern research.[19] These advancements underscore a paradigm shift in how laboratories operate, offering unparalleled opportunities for innovation.[18] Recent developments demonstrate how embedding advanced AI techniques, such as deep learning, active learning, and Bayesian optimization, into automated platforms transforms static laboratory workflows into dynamic, autonomous experimentation systems. AI technologies are increasingly capable of handling complex tasks that were traditionally manual, such as decision-making, problem-solving, and real-time adaptation.[20] Automation, on the other hand, focuses on optimizing repetitive, high-volume tasks with minimal human intervention.[17,18] The convergence occurs when AI is embedded within automated systems, allowing machines not only to perform tasks autonomously but also to learn from data, adapt to changing parameters, and improve their performance over time.[15,21]

Building on these technological foundations, we now turn to the robotic platforms and AI models that embody these principles in practice. Robotic platforms like Adam,[22] Chemputer,[23] Ada,[24] and CRESt[25] have transformed materials research, as they autonomously plan, execute, analyze, and iteratively optimize experimental procedures without constant human intervention. Here, we present a progressive roadmap (Figure 1A) to summarize achievements in both AI-informed discovery and automation-empowered synthesis. Significant progress has been made in the development of automated robotic platforms for controllable synthesis; these robotic platforms include an organic-synthesis robot,[26] modular-flow platform,[1] mobile robotic chemist,[6] high-throughput robotic platform,[27] an autonomous portable platform,[28] data-driven robotic platform,[18] AI chemist,[29] and Coscientist.[30] For unnamed technologies, such as modular-flow platform, we have adopted the most appropriate terms to represent these technologies for ease of discussion. AI models that simultaneously support robot synthesis for rational design and inverse design involve deep neural networks and symbolic AI,[31] chemical programming language,[23] synthesis-planning program,[1] Bayesian optimization,[6] synthesis literature execution,[32] closed-loop optimization,[33] computational "brain,"[29] and large language models (LLMs).[30] All these platforms and models represent significant progress in robotic platforms and even the potential of embodied intelligence-enabled synthesis.

Building upon these platforms, recent intelligent autonomous strategies have demonstrated how AI elevates laboratory automation from static execution to dynamic learning and optimization. Examples include A-lab,[21] RoboChem,[37] and Synbot,[38] which represent the next step in the evolution of AI-based synthesis, where the integration of AI not only supports but enhances autonomous decision-making and learning.[15] Specifically, deep-learning algorithms have enabled the discovery of efficient and stable crystals,[39] while the integration of robots with active learning has been adopted to synthesize computationally predicted formulas.[21] Additionally, combined software and hardware platforms have been used to determine the optimal substrate-specific conditions for photochemical processes in a scalable flow-based architecture.[37] Moreover, the development of cloud-based, delocalized, asynchronous, closed-loop discovery strategies has further advanced organic laser-emitter planning by central AI.[7] Moreover, LLMs have enabled the autonomous design and execution of laboratory experiments.[30] The convergence of generative machine learning, computer-aided synthesis planning, robotic automation, and iterative design-make-test-analyze (DMTA) cycles is now central to the development of autonomous chemical-discovery platforms, showing how AI's dynamic capabilities are reshaping the landscape of materials research. These studies also demonstrate how the embodied intelligence capabilities of hardware and AI models facilitate rational design, controllable synthesis, and inverse design.[34] Lab automation is finding increasing application in various laboratory processes.[34,37,40] Table 1 summarizes the progressive levels of intelligence in materials-synthesis laboratories, drawing comparisons with other fields such as self-driving cars,[41] unmanned systems,[42] clinical laboratories,[4] and synthetic biology.[43] It highlights the transition from basic automation to fully AI-integrated laboratories, where advanced human-robot collaboration enhances efficiency and decision-making.

Despite these achievements, a coherent review of the unified framework that connects disciplinary insights across rational design, synthesis, and inverse modeling with recent advances in automation and autonomy remains scarce. To date, high-quality reviews have explored scientific discovery with AI,[20] knowledge-integrated machine learning for materials,[44] automation and computer-assisted planning,[14] material intelligence propelled by machine learning,[45] nanoparticle synthesis assisted by machine learning,[46] and self-driving laboratories for chemistry and materials science.[47] However, few researchers have concentrated on critical reviews of the crossover of materials disciplines (e.g., rational design, controllable synthesis, and inverse design) with interdisciplinary research (e.g., data-driven science, automation, and autonomy) and the further convergence of these disciplines into contemporary research on materials synthesis. Moreover, with the advancement of automation in synthesis and data-driven robotic platforms, the evolution of materials synthesis and significant progress have been made in most recent years. This review aims to address these gaps by providing a comprehensive, interdisciplinary framework for material intelligence that systematically bridges materials science with AI and robotics through three interlinked domains of data-guided rational design, automation-enabled controllable synthesis, and autonomy-facilitated inverse design. Here, rational design, controllable synthesis, and inverse design of materials are identified as domain-specific scientific problems, while database, robotics, and embodied intelligence are the key components that shape the future of the entire field of material intelligence.[7,21,30,48] In Figure 1B, we present a comprehensive framework to organize these interdisciplinary advances, advancing material intelligence. We examine three pivotal areas (Figure 1C): data-guided rational design (extraction, "reading"), automation-enabled controllable synthesis (execution, "doing"), and autonomy-facilitated inverse design (evolution, "thinking"). The proposed reading-doing-thinking framework was deliberately chosen to illustrate the iterative, cyclic nature of material intelligence, reflecting a continuous refinement loop rather than a linear progression. This arrangement explicitly emphasizes human-AI collaboration, aligning closely with established cognitive models of scientific reasoning. Specifically, thinking informs new cycles of reading by updating databases through inverse design, while doing provides experimental validation and generates fresh insights, thus creating an adaptive, closed-loop environment. While this structure echoes the extraction-execution-evolution concept in Figure 1C, it reflects the AI-robot-scientist collaboration in practice. Reading represents data extraction and understanding, doing represents robotic execution, and thinking encapsulates reasoning and closed-loop optimization. This cyclic loop is core to our vision of intelligent, self-evolving materials research and forms the backbone of this review, illuminating the synergies among experimental, theoretical, software-driven, and data-driven paradigms. We conclude by identifying key perspectives and challenges related to designing and synthesizing advanced materials by AI and robotic platforms.

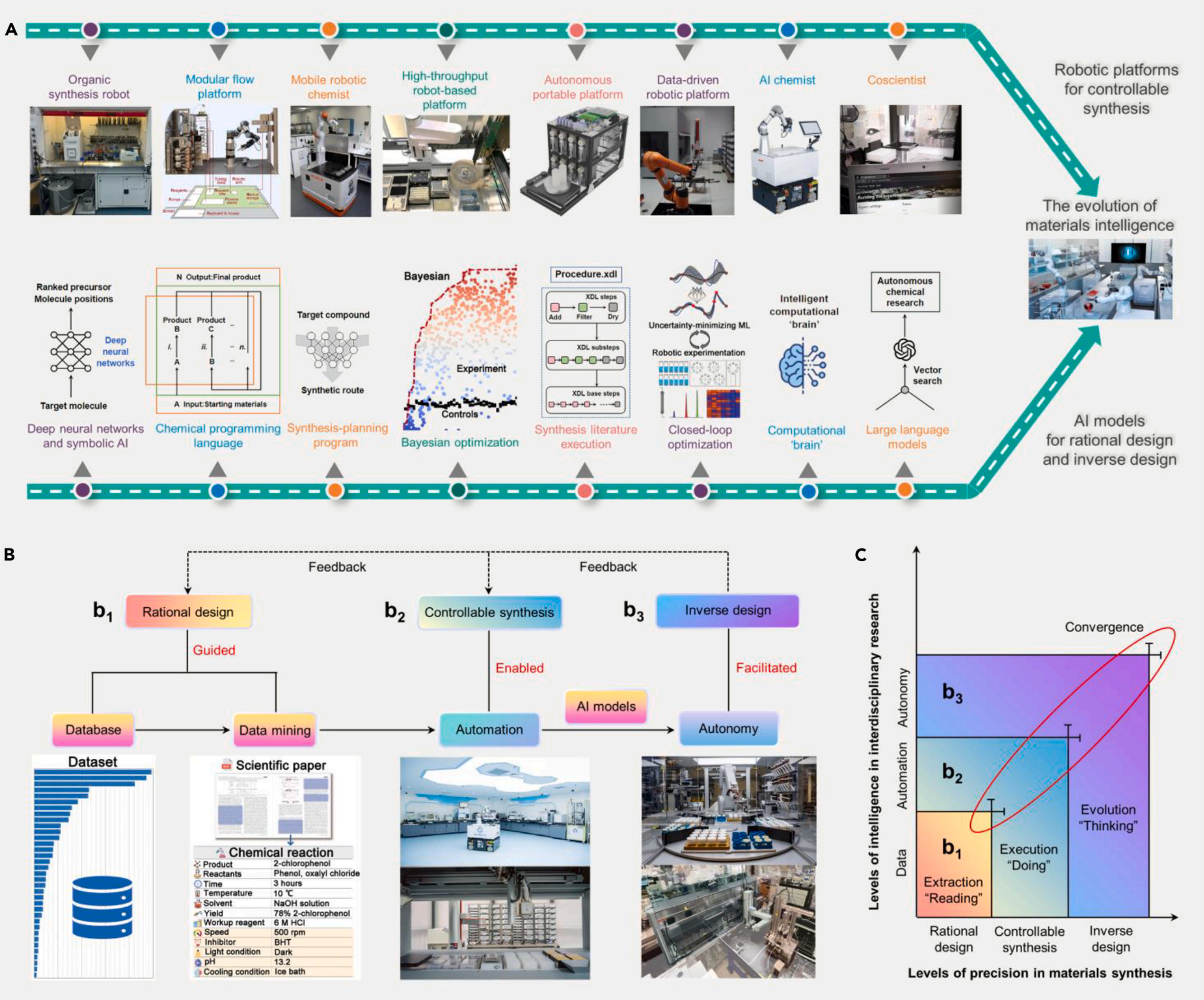

Figure 1. Progress for the integration of robotic platforms with AI models for autonomous experimentation and framework of material intelligence

(A) Development of robotic platforms (top): organic synthesis robot,[26] modular-flow platform,[1] mobile robotic chemist,[6] high-throughput robotic platform,[27] autonomous portable platform,[28] data-driven robotic platform,[18] AI chemist,[29] and Coscientist.[30] The development of AI models for robotic synthesis (bottom): deep neural networks and symbolic AI,[31] chemical programming language,[23] synthesis-planning program,[1] Bayesian optimization,[6] synthesis literature execution,[32] closed-loop optimization,[33] computational "brain,"[29] and LLMs.[30]

(B) AI model-guided rational design[30] (b_1) (rational design supported by database and data mining). Automation-enabled controllable synthesis[18] (b_2). Autonomy-facilitated inverse design[21,34] (b_3).

(C) Illustration of the integration of intelligence in interdisciplinary research and precision in materials synthesis (as data, automation, and embodied intelligence continue to evolve, the levels of intelligence in interdisciplinary research are progressively increasing. Concurrently, through rational design, controllable synthesis, and inverse design, the levels of precision in materials synthesis are steadily improving. The elliptical red circle in the figure represents the convergence and integration of computer science and materials science).

Adapted with permission from (A) (top, from left to right), ref.,[6,18,26,28–30] Springer Nature Ltd.; ref.,[1] AAAS; ref.,[27] Joule. (A) (bottom, from left to right), ref.,[6,29–31] Springer Nature Ltd.; ref.,[1,23,32,33] AAAS. (b_1) (left), (b_2) (top), (b_2) (bottom), (b_3) (top), ref.,[18,21,29,35] Springer Nature Ltd.; (b_3) (bottom), ref.,[34] AAAS; (b_1) (right), ref.,[36] Association for Computational Linguistics.

READING: DATA-GUIDED RATIONAL DESIGN

Rational design, the cornerstone of material intelligence, is a systematic methodology that leverages structure-property relationships and data-driven strategies to develop novel materials with predefined, tailored properties. Enabled by the rapid expansion of scientific data (e.g., Materials Genome Initiative[49]), this approach bridges theoretical predictions with experimental validation through four key scientific paradigms: (1) experimental data collection,[50,51] (2) theoretical simulations and computational modeling,[51,52] (3) hybrid experimental-theoretical methodologies with synthesis parameters and density functional theory (DFT) structural features,[53] and (4) data-driven informatics supporting open knowledge sharing.[54] At the core of this framework lie three interdependent pillars: (1) reliable database construction under diverse scientific paradigms (Figure 2), (2) effective data mining to extract actionable knowledge (Figure 3), and (3) adaptive AI models for predictive validation and high-throughput screening (Figure 4). Together, these components establish a closed-loop system where data continuously refine the design process, overcoming traditional limitations of scale and human bias. This section explores how these elements collectively advance data-guided rational design, with a detailed summary of the simultaneous changes in rational materials design presented in Table S1.

Beginning with data acquisition, expansive and reliable database construction under diverse scientific paradigms provides accessible

Table 1. Levels of intelligence in materials-synthesis laboratories with comparisons of self-driving cars,[41] unmanned system,[42] clinical laboratory,[4] and synthetic biology[43]

Self-driving cars[41]	Unmanned system[42]	Clinical laboratory[4]	Synthetic biology[43]	Materials-synthesis laboratory	Description	Levels
Full driving automation	Autonomous	Total laboratory automation	Machine investigator	Full AI-integrated laboratory	Fully autonomous laboratories with AI seamlessly integrated, enabling self-learning, autonomous decision-making, and real-time adaptability. Human input focuses on strategic oversight, fostering collaboration between automation and human intelligence for unparalleled precision and efficiency	5.0
High driving automation	Human aided	Serum working-station automation	Highly autonomous investigation	Partial AI-integrated laboratory	Incorporating AI into automated laboratory to drive decision-making. Accuracy of the AI model to generate decisions is still limited due to quantity and quality of input datasets	4.0
Conditional driving automation	Human directed	Task targeted automation	Conditional autonomy	Laboratory automation	A group of automated equipment is integrated in laboratory for the fully automated experimental process. Humans will set experimental goals and results will be collected	3.0
Partial driving automation	Tele-operation	Virtual automation	Partial autonomy	Equipment automation	Experimental equipment is fully automated, where processing of experimental samples by batch can be left unattended. However, manual operation is still required between experimental batches	2.0
Driver assistance	Remote control	Analytical automation	Investigator assistance	Partial equipment automation	Experimental equipment has one or two automation functions, and manual operation is highly needed	1.0

Levels of intelligence ↑

support for rational design.[20,45] The traditional method for designing novel materials is through experiments that involve high levels of human intervention.[18,29] The above samples are subjected to synthesis and characterization, leading to the creation of libraries of single-atom catalysts[50] (Figure 2A). While accurate and valuable, such datasets are limited in scale due to practical constraints. In contrast, theoretical simulations have emerged as promising alternatives, providing a broader scope and better consistency of generated data. The theory paradigm is supplemented with physical information from quantum-chemical simulations,[44] such as DFT calculations of host crystal and defect system properties[52] (Figure 2B). However, current theoretical frameworks often fall short of fully capturing the quantitative characterization requirements of materials,[20,44] calling for a hybrid experimental-theoretical database structure. For example, a database covering the electronic structure properties of more than 14,000 experimentally synthesized metal-organic frameworks (MOFs) has been used in training to rapidly and accurately predict bandgaps[51] (Figure 2C). This model extends across diverse material classes—metals, ceramics, alloys, glasses, two-dimensional (2D) materials and nanocomposites—covering materials properties like structures, formation energetics, thermodynamic phase diagrams, and electrical and mechanical properties.[44,45] To improve systematization for rational materials design, it is key to establish an open-access and standardized database, such as those for perovskite solar cells, to address global research challenges in interoperability, visualization, and interactive access[54] (Figure 2D). The most promising solution lies in developing integrated multi-fidelity databases that combine experimental data, high-level calculations, and machine-learning-generated datasets.[9] These databases support both comprehensive data mining and predictive modeling across vast compositional spaces with minimal experimental inputs. Major initiatives are already demonstrating this promise. The Materials Project,[60] Open Catalyst Project,[61] and NOMAD repository[62] collectively host millions of calculated and experimental material properties, forming the essential infrastructure for modern

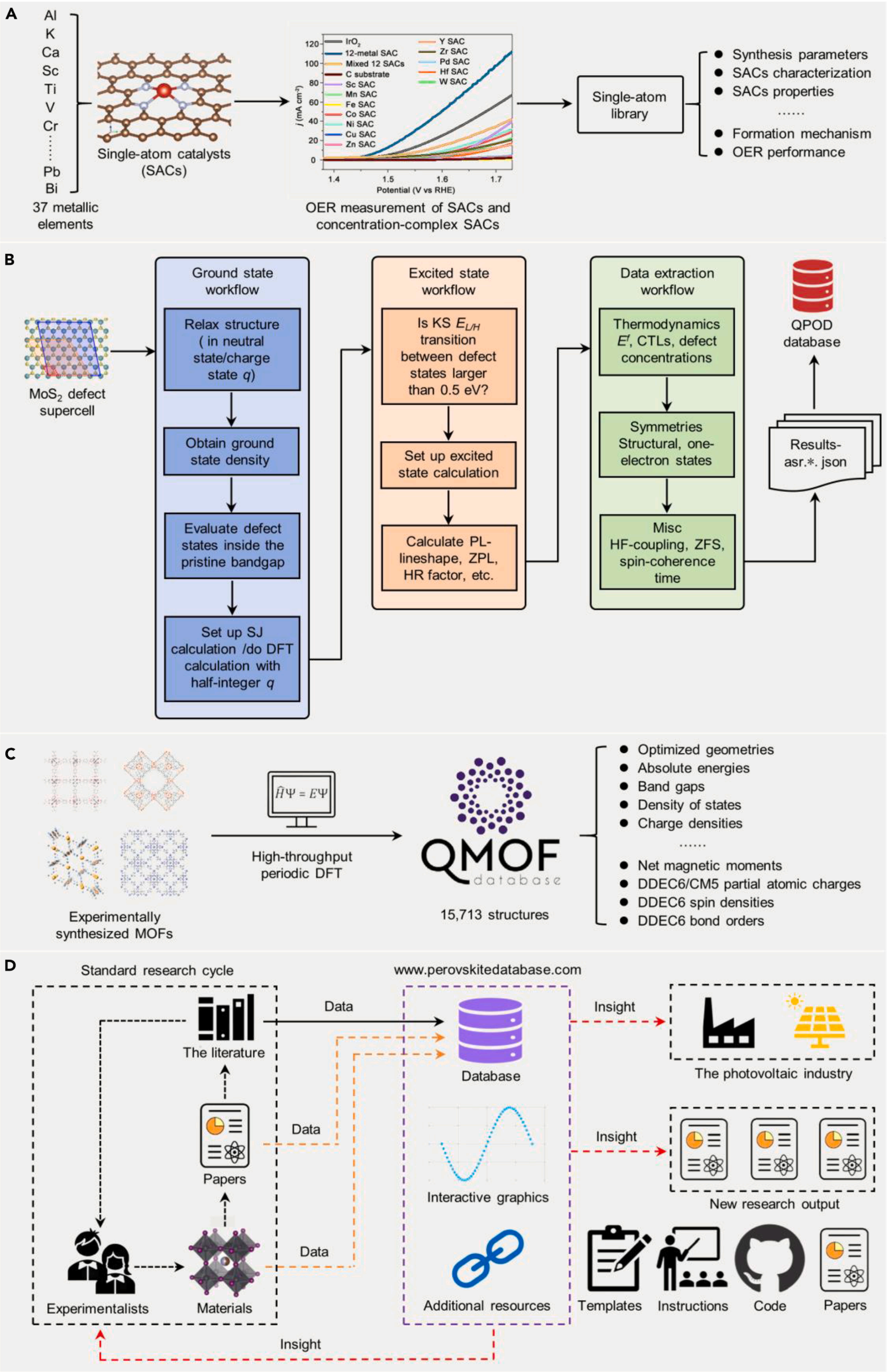

Figure 2. Database construction under the four scientific paradigms (experiment, theory, combination, and data-driven science)

(A) Single-atom catalyst experimental library.[50]

(B) Quantum point defect (QPOD) theoretical database for 2D materials.[52]

(C) Computed electronic structure-property database for experimentally synthesized MOFs.[51]

(D) Data-driven analysis tool for perovskite solar cells.[54]

Adapted with permission from (A, B, and D) ref.,[50,52,54] Springer Nature Ltd.; (C) ref.,[51] Matter. OER, oxygen evolution reaction; SJ, Slater-Janak theorem; DFT, density functional theory; KS, Kohn-Sham electronic states; PL, photoluminescence; ZPL, zero phonon line; HR, Huang-Rhys; CTL, charge transition level; HF, hyperfine coupling; ZFS, zero field splitting; MOFs, metal-organic frameworks.

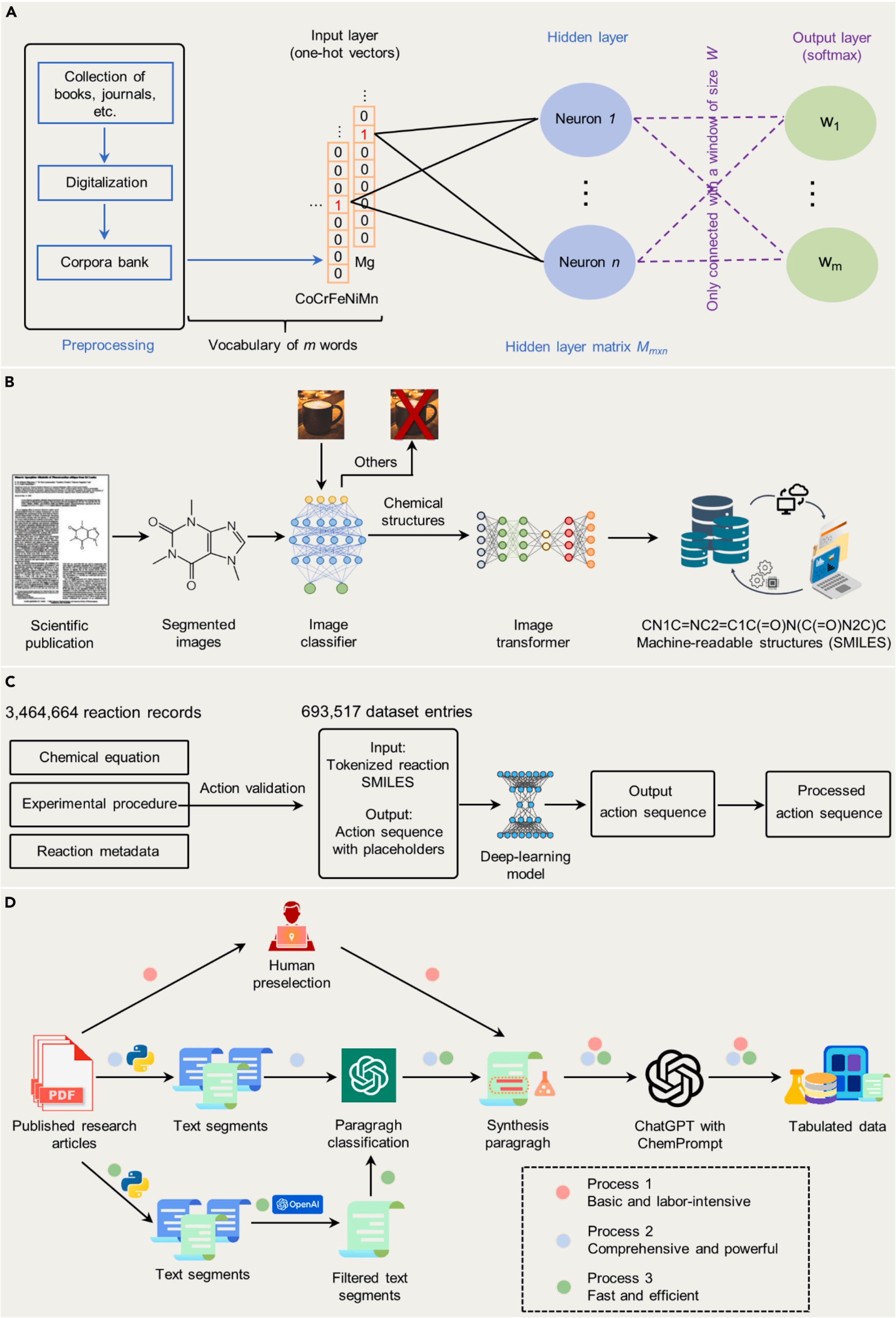

Figure 3. Development of data mining for chemical elements, structures, reactions, and knowledge discovery
(A) Selection of chemical elements for ultrahigh-entropy alloys.[55]
(B) Chemical structure detection, segmentation, and interpretation in scientific literatures.[56]
(C) Synthesis procedure inference from text-based representations of chemical reactions.[57]
(D) GPT Chemistry Assistant for MOF synthesis parameters and crystallization prediction.[53]
Adapted with permission from (A–C) ref.,[55–57] Springer Nature Ltd.; (D) ref.,[53] ACS.

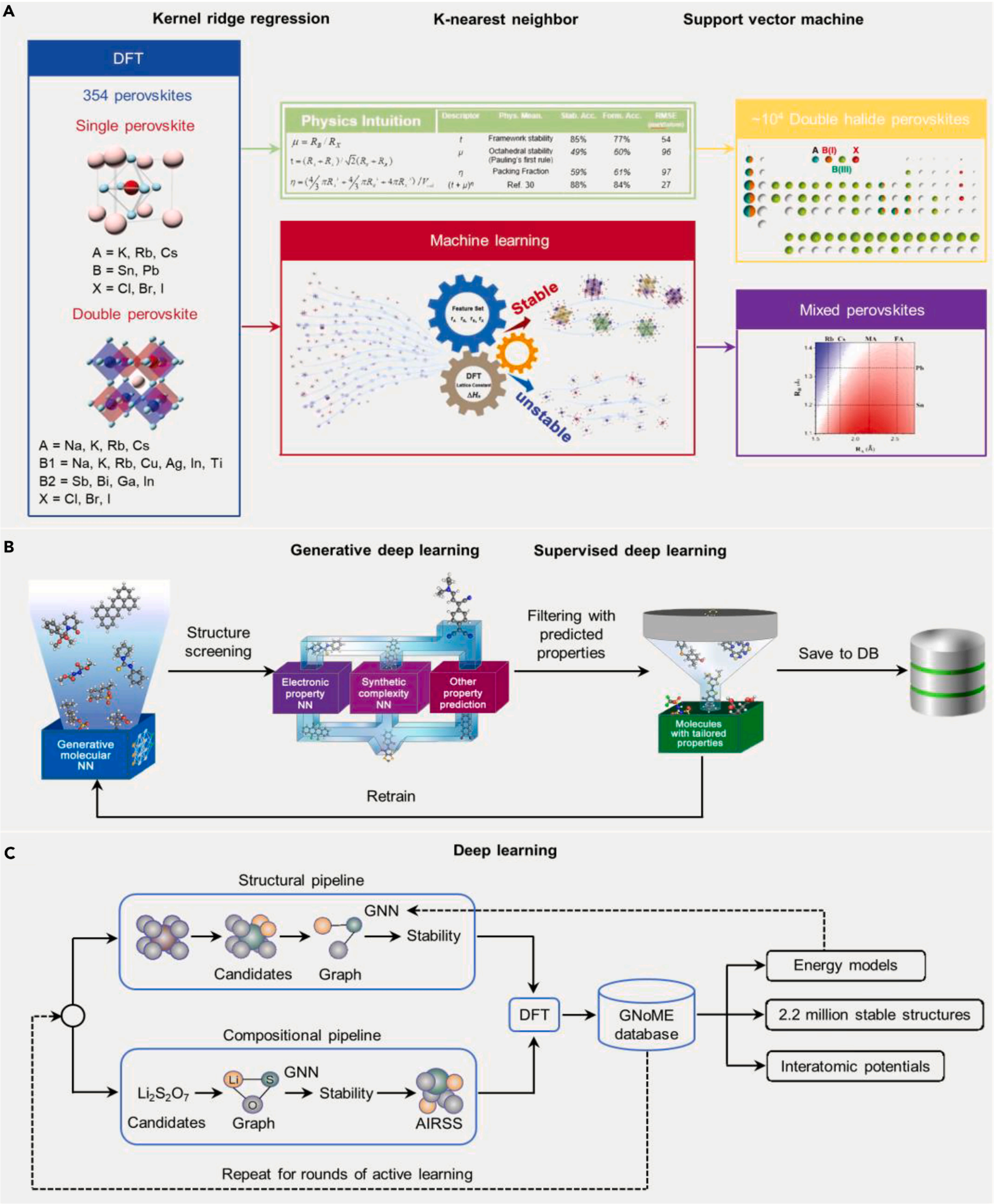

Figure 4. AI models for result validation, high-throughput screening, and rational materials design

(A) Thermodynamic stability validation of halide double perovskites.[58]

(B) High-throughput property-driven screening of functional organic molecules.[59]

(C) Deep-learning algorithms for stable crystal design.[39]

Adapted with permission from (A) ref., Wiley; (B and C) ref.,[39,59] Springer Nature Ltd. NN, neural network; DB, database; GNN, graph neural network; AIRSS, *ab initio* random structure searching; DFT, density functional theory; GNoME, graph networks for materials exploration.

material informatics. These resources have enabled remarkable advances in machine-learning applications, for instance, graph neural networks (GNNs) trained on these datasets achieve over 90% accuracy in predicting formation energies.[39] Similarly, GNNs trained on nanomaterial databases can predict optimal drug-carrier formulations with over 80% accuracy, reducing the number of experimental screenings in biomedicine.[63] Foundation models like DARWIN[64]—a domain specific LLM for Natural Science—further enhance this framework by enabling efficient knowledge transfer across material classes through pre-training on extensive chemical databases. By harmonizing high-quality experimental data with computational results and machine-learning-generated insights, these next-generation databases are poised to fundamentally transform the capabilities of rational materials design.

Second, building upon these database infrastructures, effective data-mining techniques serve as a crucial bridge between raw data and practical applications in rational design. By extracting actionable insights from vast datasets, these methods enable systematic analysis of key factors such as chemical elements,[55] structures,[56] reaction pathways,[57] and knowledge,[53] which are potentially attractive tools and methods for accelerating rational design.[20] Regarding data standardization, inherently machine-readable computational data are readily mined from database/platforms such as the Materials Project,[60] Automatic FLOW for materials discovery (AFLOW),[65] and Open Quantum Materials Database (OQMD).[66] Experimental data, however, pose challenges due to inconsistent historical data reporting, with manual data extraction being error prone and labor intensive. Advanced algorithms address this issue through literature mining, identifying trends, relationships, and knowledge gaps from extensive corpora (for instance, uncovering alloying elements for rational alloy design[55]) (Figure 3A). In molecular materials discovery, schematic representations are widely used to illustrate information alongside simple text.[45] These schematics are mined via optical chemical structure recognition, converting diagrams into machine-readable formats[56] (Figure 3B). Beyond structures, Figure 3C demonstrates the inference of experimental procedures from text-based representations of chemical reactions.[57] Together, these methods contribute to a more automated and scalable approach to materials synthesis planning, potentially accelerating synthesizability evaluation for the automated driving and general-purpose synthetic chemistry of robotic systems.[14] Computational planning enhances this approach by addressing complex synthesis challenges, as demonstrated with natural products using advanced algorithms to optimize synthetic pathways, thereby significantly improving both the efficiency and feasibility of complex molecule synthesis within automated platforms.[67] Knowledge discovery, intertwined with rational design, uncovers hidden patterns to guide scientific innovation. Data-driven insights gained from knowledge discovery directly inform systematic approaches to material innovation and process optimization.[68] By revealing underlying patterns and trends, knowledge discovery enables more informed, systematic approaches to designing new materials or processes.[44] Recently, LLMs, e.g., DARWIN,[64] LS-GenAI,[69] MatChat,[70] and PolyNC, have transformed this landscape.[71] These models significantly accelerate material discovery by harnessing LLMs to analyze extensive datasets, uncover patterns, and generate predictive insights.[45] For instance, LLMs contribute to the creation of knowledge-based synthesis conditions for MOFs and the prediction of crystallization outcomes[20] (Figure 3D). These tools range from semi-automated processes requiring human input to fully autonomous systems with embedded filtering, enhancing speed and efficiency. Figure 3D process 1 requires human intervention for the identification and extraction of synthesis sections from literature. Process 2 achieves full automation by integrating classification and summarization into a seamless pipeline. Process 3 is the most efficient, which incorporates embedding-based section filtering to minimize classification complexity and maximize throughput.

The third key pillar, building upon the foundation of data mining and database construction, lies in the application of AI models for result validation,[58] high-throughput screening,[59] and rational materials design.[39] For example, thermodynamic stability has been used to validate machine-learning predictions derived from theory-based databases, providing a unique opportunity for addressing fundamental questions about perovskite applications, closely aligning with experimental observations[58] (Figure 4A). AI models enable large-scale, efficient, high-throughput screening processes to identify high-potential candidates suited for targeted applications. Property-driven generative design has shown the ability to perform multi-objective high-throughput screening of functional organic molecules, accelerating the optimization of material properties[59] (Figure 4B). Moreover, deep-learning algorithms have expanded the possibility of exploring potential solutions within the field of materials science, enabling the accurate simulation and prediction of materials discovery process results.[44,45] Notably, the materials field has witnessed particularly significant progress through three landmark AI architectures: (1) GNoME achieves unprecedented accuracy in inorganic materials discovery, with 11 meV/atom mean energy error and over 80% precision in stable material identification, while demonstrating exceptional generalization to five-element systems beyond its training domain[39] (Figure 4C); (2) MatterGen combines high uniqueness (86% at 1 million samples) with novel stable structure generation (68% novelty), showing close DFT alignment and effective extension to high-entropy alloys[72]; and (3) AlphaFold 3 revolutionizes interface prediction with significant error reduction versus conventional docking tools while maintaining generalization across post-translational modifications and small molecules.[73] Together, these innovations reflect a trend toward increasingly integrative systems. Looking ahead, the field is set to progress toward more powerful, integrative systems.[21] The next frontier likely involves multi-modal learning, combining chemical, electronic, and structural data to generate more comprehensive material models.[44] Additionally, with improvements in model interpretability, AI systems will move from prediction to actively guiding experimental workflows and material synthesis.[9] These advancements will pave the way for automated, generative systems capable of rapidly designing and optimizing materials for diverse applications.[29] Furthermore, the integration of sustainable practices in data-guided rational design can significantly reduce the environmental footprint of materials discovery. By leveraging AI to optimize resource-efficient pathways and minimize waste, this approach aligns with the principles of green chemistry and sustainable development.[9]

As a culmination of these developments, Figure 1B illustrates the changes in data-guided rational design demonstrated by the improved ability of database construction, data mining, and advanced AI models for actionable applications in the era of data-rich research.[20,45] Extraction reading reflects the collection and analysis of data: the organization of domain-specific datasets into well-constructed databases provides machine-readable, standardized access to information for the automated extraction and processing using computational tools,[57] allowing for building comprehensive understanding using modern statistics for data analysis and, moreover, for AI models to draw from large databases to extract patterns and refine approaches based on previous experiments.[39] This progression enables AI-driven models to learn from datasets on material formula, synthesis parameters, and experimental outcomes.[9] With standardized, high-quality, large-volume database as the foundation, data mining using statistical tools enables an efficient grasp of correlations across high-dimensional space, ultimately empowering an AI-driven, automated approach to accelerating the rational and inverse design of materials.[15] This transformation has redefined the reading stage of scientific discovery—enabling scientists to derive insights at a depth and scale far beyond human capacity and guiding automated, knowledge-informed experimental planning.[44] The future of automation in materials design will likely be hinged on the continuous evolution of advanced technologies such as LLMs, multimodal learning, and quantum computing.[74] These innovations promise to push AI models from passive pattern recognition to deeper insights and faster discoveries in materials science.[20,75] However, challenges persist: current high-volume databases are predominantly computation based,[52] while the experiment-based literature data suffer from inconsistent reporting and human biasing.[3] This mismatch restricted our ability to establish comprehensive links between the real-world materials challenges and *in silico* simulations,[51] and the current limitation lies in how to narrow the scope of screening while producing reliable results,[44] highlighting a significant need for precise and controllable materials-synthesis systems. As outlined in this section, the extracted knowledge in this reading stage forms the computational foundation that enables real-world application through thinking and doing.

DOING: AUTOMATION-ENABLED CONTROLLABLE SYNTHESIS

Automation represents the critical bridge between data-guided rational design and controllable synthesis in material intelligence. Controllable synthesis traditionally relied on manual trial-and-error experimentation and chemical evaluation involving weighing, mixing, heating/cooling, separation, and purification to achieve specific material properties,[17,18] but it suffers from inherent inconsistencies due to human variability in expertise and workflow execution.[17,29] Modern robotic platforms overcome these limitations by automating complex processes—from reagent dosing to *in situ* characterization—while enabling unprecedented control over materials components,[29] structures,[26] morphologies,[18] and processes,[27] which enhance reproducibility and enable high-throughput synthesis. Within automation-enabled controllable synthesis, three primary aspects are emphasized: (1) robotic platforms

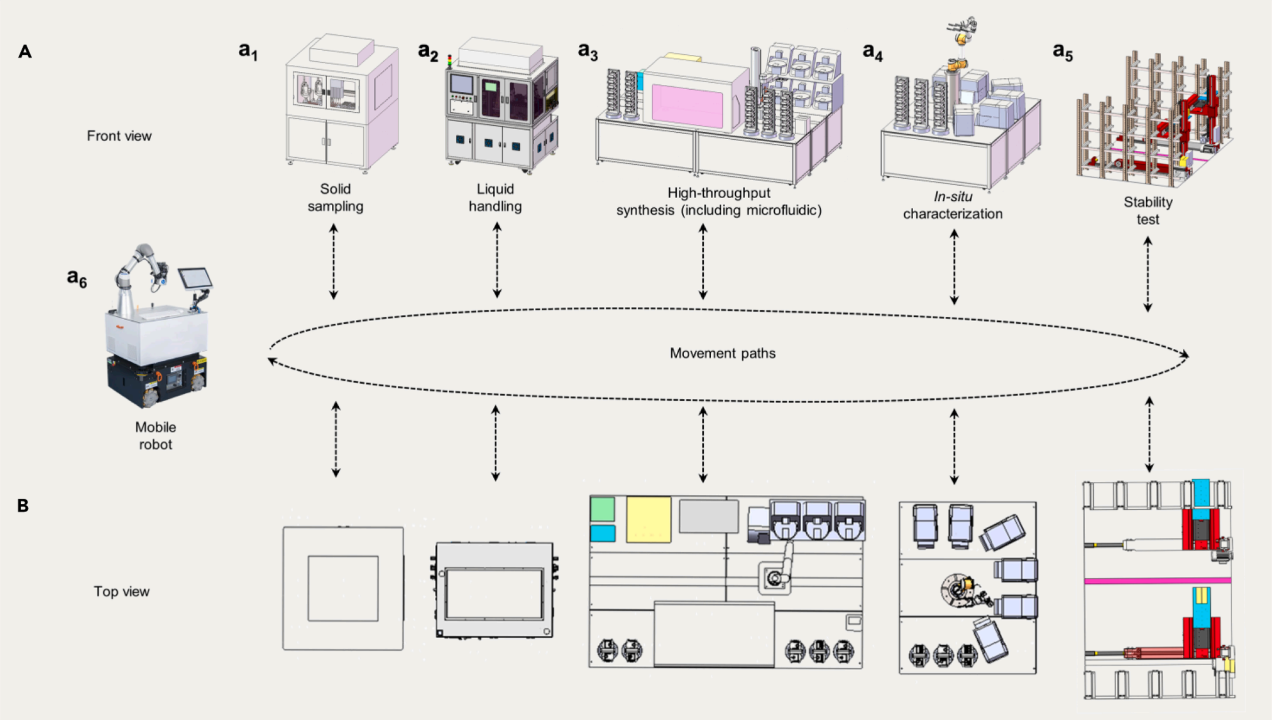

Figure 5. Illustration of robotic platform and modules for controllable synthesis

Front view (A) and top view (B) of robotic-platform modules with mobile robots to link the experimental modules.[18] The diverse modules have specific functions for (a_1) solid sampling,[6,21,38] (a_2) liquid handling,[79–81] (a_3) high-throughput synthesis (including microfluidics),[6,7,27,29,82] (a_4) *in situ* characterization,[19,29,84] (a_5) stability test,[6,29] and (a_6) mobile robot for interconnection.[6,29]

tailored for different synthesis needs, (2) high-throughput synthesis strategies for batch and flow systems, and (3) *in situ* characterization and integration techniques for system optimization and safety. This section systematically explores these components, highlighting how they collectively enable the execution, doing phase of material intelligence.

Recent advancements in programmable robotics have allowed the execution of complex controllable synthesis processes,[2,76] yet challenges persist in cross-platform reproducibility due to disparities in equipment calibration, reagent purity, and software algorithms.[15,16] To address this, emerging strategies include real-time environmental monitoring,[37] standardized calibration protocols,[30] and the integration of digital twins for centralized benchmarking.[16] In addition, establishing universal benchmarking standards is instrumental in quantifying and evaluating the reproducibility and scalability of automated systems.[8,19,26,77] Key metrics such as synthesis yield, throughput, data quality, and variance in product properties, together with robotic performance indicators such as accuracy and cycle times, provide a foundation for assessing reliability and scalability of automated robotic systems.[32] By integrating these reproducibility-focused strategies and robust benchmarking standards, automated robotic platforms are poised to deliver scalable, efficient, and reliable solutions for controllable synthesis.[78] To explore this further, this section explores how automation transforms controllable synthesis, focusing on robotic platforms, high-throughput synthesis, and *in situ* characterization.

Building on this foundation, robotic platforms for controllable synthesis vary widely in design and functionality, each exhibiting distinct advantages and limitations tied to their operational paradigms. For instance, solid-handling systems like A-lab enable high-throughput inorganic materials discovery with 71% success rate through automated powder processing and real-time characterization validation, yet they are constrained by predefined compositional libraries and air-sensitive materials.[21] In contrast, liquid-handling platforms such as Chemputer excel in modular organic synthesis but struggle with heterogeneous systems due to particulate clogging and limited solid-liquid interface control.[23] Emerging LLM-driven experimentation systems like Coscientist demonstrate broad hypothesis generation potential but often propose synthetically infeasible protocols requiring human intervention.[30] This divergence in capabilities underscores the need for platform selection aligned with target material classes for practical materials discovery (e.g., solid-state synthesis favors A-lab's precision, solution-phase chemistry aligns with Chemputer's flexibility, while hypothesis generation benefits from Coscientist's broad knowledge integration). These robotic transforms AI-generated rational design hypotheses, translating modeling outputs into material synthesis with enhanced precision, reproducibility, and scalability. For example, Chemputer and A-lab systems have demonstrated the ability to autonomously execute complex synthesis protocols derived from computational predictions.[21,23] Digital twins further reinforce this link between simulation and practice by pre-validating experimental setups under realistic conditions. These technologies enable a direct and iterative connection between data-driven modeling and real-world material fabrication.

Generally, these robotic platforms can be categorized into modular systems for solid sampling,[6,21,38] liquid handling,[79–81] high-throughput synthesis (including microfluidics),[6,7,27,29,82] *in situ* characterization,[3,17,19,83] stability testing,[19,29,84] and mobile interconnected robotics[6,29] (Figure 5). To provide a visualization of the overall system, the front view (Figure 5A) and top view (Figure 5B) of a standard robotic platform interconnected via a mobile robot are presented for illustration.[18] Automated synthesis often begins with precise reagent dosing, with solid dosing that involves handling and measurement of powders or granules[21] and liquid dosing that requires precise volume control and mixing of liquids.[79] Solid sampling robots excel at handling powdered materials for reagent dosing and are crucial for processes involving catalysts and nanoparticles.[80] For instance, solid sampling robots have been employed for diverse applications, including the automated extraction of hydrogen from water via robotics (688 experiments),[6] the automated synthesis of oxygen-producing catalysts from Martian meteorites by a robotic AI chemist (3,764,376 formulas),[29] and the automated synthesis of organic molecules through AI-driven robotic chemists (12 reactions).[38] Notably, A-lab platform further exemplifies advanced integration, combining solid dosing with active-learning algorithms and real-time X-ray diffraction analysis to prioritize synthesis targets.[21] Through this iterative optimization protocol, A-lab is able to achieve autonomous synthesis of 41 target inorganic materials from 58 candidates within 17 days of continuous operation. Despite their effectiveness, solid sampling robots may lack the homogeneity and precision achievable in liquid-based systems for solution-phase reaction.[21] In comparison, liquid-handling robots revolutionize solution-based chemistry, enabling breakthroughs in combinatorial chemistry,[11] thin-film materials synthesis,[79,85] drug discovery,[1,26] and automated microfluidic platforms for performing systematic studies on colloidal perovskite nanocrystals for continuous nanomanufacturing.[82] With a precise robotic processing system, it has assisted the exploration and optimization of nanomaterials discovery via chemical synthesis robots (1,000 experiments)[80] and non-aqueous Li-ion battery electrolytes via robotic experimentation (6-fold acceleration).[81] Advanced implementations like ChemOS coupled these robotic liquid handlers with flow reactors and online analytics, using reinforcement learning to optimize photoredox reactions in fewer than 10 experimental iterations.[86] However, while liquid-handling systems are indispensable for solution-based synthesis, they lack the versatility required for solid-state reactions and heterogeneous systems.[81] Furthermore, it would be challenging for liquid-handling systems to be applied to highly viscous liquid, especially for formulations.[21] Given these limitations, the development of a general-purpose reagent dosing (or reaction preparation) system is a pressing need.[6] Key concerns include multi-scale operations (nanogram to gram scale), challenging formulations (viscous liquids, slurries, low/high temperatures, inert environments), and an automated stock-management system.[3]

Beyond the dosing process, high-throughput synthesis platforms further support materials discovery with controllable properties via batch or flow-based approaches.[1] Both batch and flow-based synthesis approaches have distinct advantages and limitations, and their suitability depends on specific material synthesis needs.[87] Batch synthesis systems, typically employed for small-scale material development, offer greater flexibility for exploring diverse synthesis parameters owing to their ease of parallelization.[77,87] However, their reproducibility can be limited by manual interventions between experimental steps.[2,8] Platforms like Chemspeed and Unchained Labs address this challenge by automating synthesis, screening, and characterization, demonstrating effectiveness in fields such as catalyst and drug development. Similarly, open-source platforms like Opentrons lower the cost barrier, enabling academic and startup researchers to adopt customizable high-throughput workflows. Advanced systems like the Chemputer[23] further exemplify how automation can enhance synthesis versatility, as it is programmed to perform a wide range of protocols and reactions. It integrates robotics with advanced chemical synthesis, aiming to transform research in chemistry and materials science by enhancing efficiency, reproducibility, and scalability in complex scientific processes.[3] In contrast to batch systems, flow-based approaches, particularly microfluidics and modular-flow platforms, excel in continuous synthesis applications.[1] Microfluidic platforms offer fine-scale control over reaction environments at the microscale, making them ideally suited for continuous and precise production of nanoparticles and pharmaceuticals.[7] For instance, the on-demand and continuous-flow production of pharmaceuticals in a compact and reconfigurable system,[77] microfluidic electrochemistry for single-electron transfer processes and redox-neutral reactions,[88] a reinforcement-learning-optimized lipid-nanoparticle platform for gene delivery,[63] a robotic platform for the flow synthesis of organic material formula informed by AI planning,[1] a plug-and-play fluidic microreactor for autonomous flow-based synthesis and optimization of quantum dots,[85] and automated microfluidic platform for performing systematic studies on colloidal perovskite nanocrystals for continuous nanomanufacturing.[82] However, despite their precision, limited reaction volumes pose a major bottleneck for industrial-scale applications.[29] To overcome this, modular-flow platforms have emerged as a scalable alternative that supports large reaction volumes and high-throughput synthesis at industrial levels. These platforms have shown breakthroughs in the development of organic photovoltaic (OPV) materials (100 processing variations),[27] stable and efficient wide-bandgap metal halide perovskite alloys (10-fold research acceleration),[89] and organic solid-state laser gain materials with top-tier lasing performance (>150,000 candidates).[7] Although they may trade off some microscale control compared to microfluidics, modular platforms enable high-throughput synthesis for large-scale production and support continuous-flow synthesis of materials at industrial levels. Combining the advantages of both, modern modular platforms are capable of performing multi-step synthesis dynamically.[29] The inclusion of new synthetic methodologies such as photo, electro, and mechanical synthesis further positions them as a core enabler of materials-on-demand platforms.[37]

Beyond synthesis, automation in material intelligence extends to testing and analysis. *In situ* characterization and stability testing provide real-time data for process optimization, providing real-time feedback during synthesis. These techniques are widely applied in the study of perovskites,[17,83,84,90] silver nanocrystals,[5] gold nanorods,[91] MOFs,[92] photocatalysts,[19] and lithium batteries,[93] enabling the monitoring of morphology and composition-dependent behaviors. Representative methods include spectroscopic measurements such as ultraviolet-visible (UV-vis) absorption,[19,90] fluorescence,[19,83] steady-state and time-resolved spectroscopy,[84,90] color characterization,[5,17] and transmission electron microscopy (TEM).[91,92] The AI chemist laboratory, for instance, integrates gas chromatography to assess catalytic performance, enhancing real-time characterization.[19] Similarly, the AutoSyn system utilizes mobile robotic arms to dynamically reconfigure reactor setups based on real-time spectral analysis data, demonstrating superior effectiveness in organic synthesis as compared to manual screening.[94] These robotic advances extend to biomaterials research, where autonomous platforms can process over 10,000 material-cell interactions daily using real-time computer vision.[95] However, the scalability of such systems depends on overcoming fragmented biocompatibility data through AI-augmented text mining to ensure reproducibility.[96] Additionally, high-throughput characterization methods such as X-ray diffraction, electrochemical testing, and synchrotron radiation further support in-depth investigations of material structures and properties.[93] As automated systems become more complex, integrating and hosting diverse robotic modules has emerged as a new challenge, especially in constrained physical spaces.[7] Integrating experimental modules with robots, such as mobile robotic chemists for photocatalysts,[6] enables platforms to link previously disconnected stages of reagent preparation, synthesis, characterization, and performance testing, thus establishing a multi-module, data-driven paradigm. This integration facilitates the efficient synthesis of new and optimized materials with desirable properties.[7,15,17] The success of such platforms relies heavily on precise motion planning, requiring algorithms to consider physical constraints, such as reach, speed, and payload capacity, while optimizing efficiency and accuracy.[30] To address this, digital twins, virtual models of physical systems, have been employed to simulate robotic trajectories, predict collisions, and optimize task sequences before physical execution.[7] Digital twins also support real-time monitoring and adaptive reconfiguration, making the paradigm more efficient and more resilient to variation.[97]

In parallel with technical capabilities, lab safety remains a foundational consideration. Robots can reduce human exposure to hazardous chemicals, high temperatures, and toxic substances.[17] Nevertheless, safe interaction between robots and human operators remains paramount.[18] Collaborative robots operating alongside researchers must be equipped with advanced safety mechanisms, including emergency stop functions, force-limiting technology, and continuous environmental monitoring.[8] In more hazardous or fully autonomous setups, safety protocols such as secure barriers, collision-detection sensors, and fail-safe protocols are essential. By integrating motion planning, digital twin simulations, and robust safety systems, robotic technologies can enhance lab efficiency while ensuring safe and effective operations.[3] Beyond physical safeguards, the autonomous nature introduces ethical imperatives that necessitate proactive governance. The delegation of experimental decision-making to AI systems, for instance, mandates rigorous validation protocols to prevent "illusions of understanding," where models produce superficially plausible but physically unsubstantiated hypotheses[98]—a risk especially crucial in high-stakes applications involving explosive precursors or biohazardous materials. Concurrently, the rise of automated laboratories underscores unresolved challenges in data ownership and reproducibility standards. Transparent benchmarking initiatives, such as FAIR (findable, accessible, interoperable, and reusable) compliant datasets[54] will be needed as it potentially addresses these concerns. Furthermore, the environmental footprint of high-throughput robotic systems, from energy consumption to solvent waste, requires deliberate integration of green chemistry principles to promote future sustainable development, as demonstrated recently by resource-optimized platforms.[37,77] Together, these technical and ethical frameworks align with emerging guidelines for responsible AI in material science, ensuring its advancement in terms of both innovation and accountability.

Collectively, the synergy between AI-driven robotic and high-throughput synthesis with real-time characterization empowers the data-driven selection of optimal synthesis parameters.[7,18,19,29] For instance, robot scientists have broadened the possibilities for translating synthesis goals into robotic actions, experimentally characterizing crystal morphologies and identifying correlations between synthesis parameters and materials properties with machine-learning models.[18]

This process aligns macro-level synthesis parameters with programmable robotic hardware and microstructure-property features, such as particle sizes, shapes, and grain-boundary pinning points, thereby facilitating the targeted fabrication of specific materials.[17,18] Additionally, tools such as XDL, a universal chemical programming language, have been developed to standardize synthesis parameters across different robotic platforms. These frameworks streamline the translation of experimental designs into machine-readable executable protocols, strengthening the link between physical experiments and digital paradigm, bolstering the precision and scalability of automated synthesis.[78] The expansion of databases and sharing of standardized protocols within the scientific community further support the design of *de novo* materials with enhanced properties and the discovery of synthesis mechanisms beyond conventional knowledge.[21] Furthermore, the integration of digital twins into synthesis parameters creates a new paradigm for materials design, merging physical and cyber systems to enable predictive and adaptive experimentation.[1,2] The combination of high throughput, high precision in controlling experimental details, and outstanding data quality contribute to digitally controllable synthesis.[78] The aspects of materials automation systems for controllable synthesis, including experimental databases, algorithms, function of software, function of hardware, performance, and applications, are provided in Table S2 for synthesizing small organic molecules,[1,2,26,31] magnetic nanographenes,[48] electrocatalysts,[99] nanocrystals,[5,18,100] and solar cells.[27]

Building on this foundation, the integration of AI models with robotic control systems in data-driven automated platforms has substantially improved the precision, efficiency, and scalability in materials synthesis, revolutionizing the field of materials science.[1,17,48] These systems enable the autonomous execution of experimental tasks under the context of execution—doing, where robotic systems perform complex synthesis guided by AI-derived insights.[18] While the role of AI is transformative, human-in-the-loop strategies remain indispensable for real-time intervention, interpretability, and adaptive feedback-based optimization.[21,34,37] This collaborative approach between automated systems and human chemists empowers the intelligent design of novel materials and the refinement of existing formulations, achieving products that meet rigorous performance standards.[21] As physical-cyber systems advance toward greater autonomous capabilities, human oversight and ethical considerations will ensure that these innovations serve the broader goals of societal well-being.[3] This synergy marks a paradigm shift in materials discovery, empowering breakthroughs in rational design, inverse design, and intelligent manufacturing while keeping humanity's best interests at the forefront.[12]

THINKING: AUTONOMY-FACILITATED INVERSE DESIGN

Autonomy-facilitated inverse design empowers AI models to interpret and execute predefined tasks and to independently generate hypotheses, plan experiments, and optimize materials. This paradigm enables machines to think through iterative closed-loop strategies that search, refine, and converge on optimal synthesis based on predefined target properties. Central to this approach is inverse design, which reverses conventional experimental logic by starting from desired functionalities and working backward to identify material formulas, synthetic routes, and environmental parameters. Moving beyond programmable workflows, self-driving laboratories now embed advanced AI agents capable of modeling, real-time reasoning, and autonomous decision-making. These capabilities are enabled by three key components: (1) model-driven and model-free optimization methods, including Bayesian inference, reinforcement learning, and generative models, that guide exploration in complex, high-dimensional parameter spaces (see Figures 6A–6C); (2) integrated modular automation platforms synchronizing software and hardware for experimental execution and feedback (see Figure 6D); and (3) digital twins that simulate and validate synthesis setups before real-world trials (see Figures 7A–7D). This section explores how such systems converge into a cohesive inverse design paradigm, delivering autonomy in materials discovery through closed-loop experimentation.

The transition from manual experimentation to fully autonomous laboratories (commonly known as self-driving laboratories) marks a transformative development in materials science.[3] At the heart of this transformation is the inverse design approach that has been adopted for material synthesis, relying on computational methods to define desired functionalities and identify the optimal material formula, synthesis parameters, and reaction conditions.[12,45] Early efforts in automation focused on repeatable, programmable paradigms, while current autonomous laboratories go further by embedding advanced AI algorithms capable of iterative learning, decision-making, and closed-loop optimization.[15] This evolution requires a new level of laboratory intelligence, which we refer to as evolution thinking, which encompasses hypothesis generation, modeling, and optimization via iterative closed-loop cycles.[30] Such embodied intelligence is driven by data integration and AI-driven decision-making, enhancing the precision of material design with minimal human input.[19] Digital twins further augment these closed-loop systems, which enable remote monitoring and simulation of experiments, refining experimental setups before real-world implementation. By simulating real-time data *in silico*, digital twins can improve the accuracy of predictions and support autonomous decision-making, which enables autonomous systems to simulate and apply validated decisions directly to real-world synthesis. This section examines how inverse design, as the apex of material intelligence, enables autonomous systems to iteratively optimize materials for target properties through closed-loop experimentation.

Building on this conceptual foundation, the realization of autonomous inverse design's full potential demands coordinated advances across multiple technological frontiers. Central to this challenge is the seamless integration of automated synthesis with intelligent decision-making, a task increasingly addressed by sophisticated methodologies capable of navigating high-dimensional parameter spaces under practical constraints, including synthesizability and cost.[7] Bayesian optimization exemplifies this progress, where Gaussian processes strategically balance the exploration of novel conditions with exploitation of promising candidates, using multi-objective acquisition functions to simultaneously optimize performance and resource efficiency.[104] Reinforcement learning extends these capabilities further, employing reward-based policies to adapt to dynamic experimental environments—from optimizing photocatalytic reactions with minimal rare-metal usage[37] to atomic-scale precision in robotic nanofabrication.[105] Complementing these approaches, generative models such as diffusion networks[72] and generative adversarial networks (GANs)[106] learn latent representations of chemical spaces to propose novel structures. Recent comparative studies reveal fundamental distinctions in these methodologies. Bayesian optimization, as demonstrated in photocatalyst development,[37] achieves sample efficiency (<100 experiments to

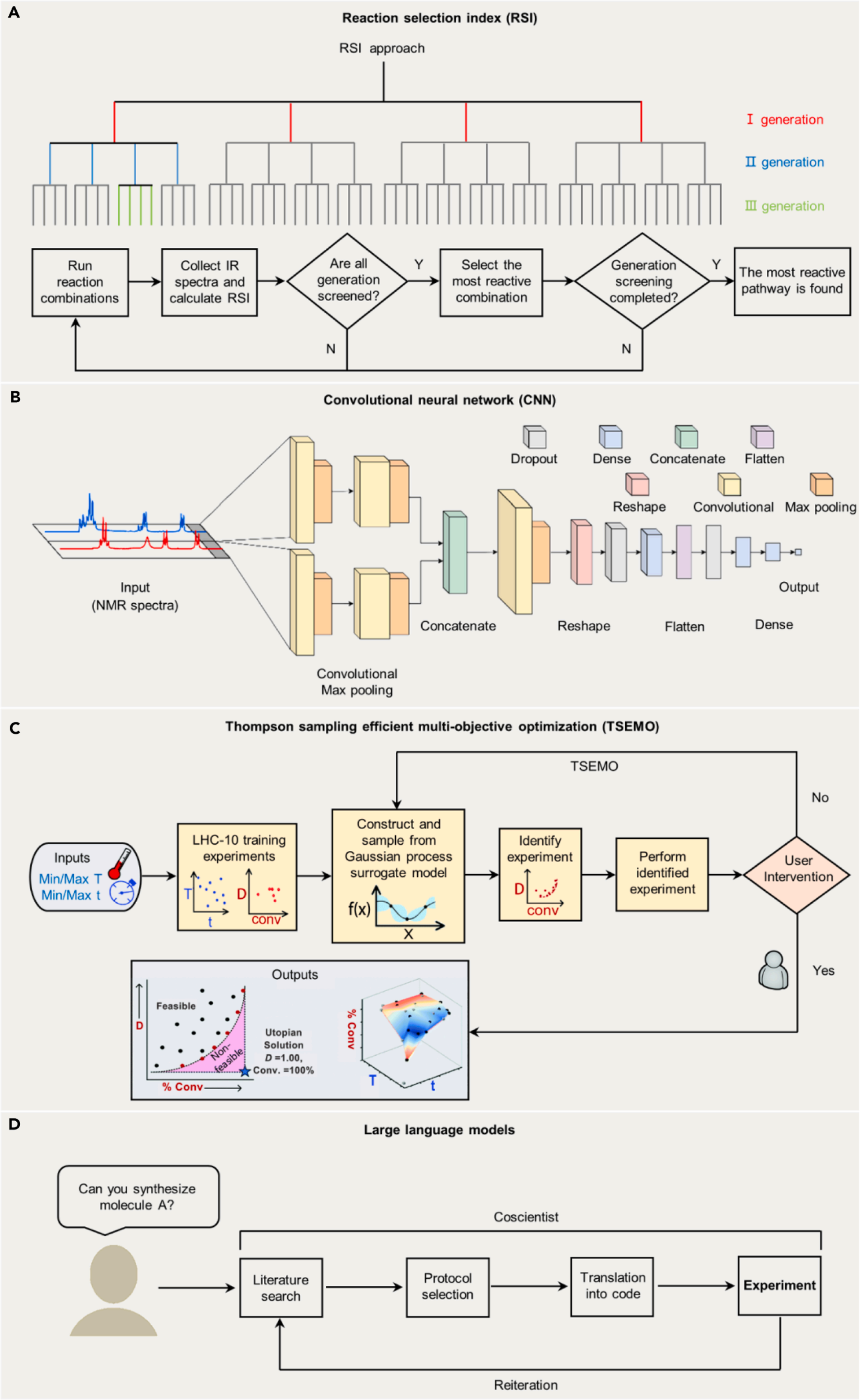

Figure 6. Revolution of autonomous synthesis by the RSI, convolutional neural network, multi-objective optimization, and LLMs

(A) Autonomous organic reaction search engine for chemical reactivity.[101]

(B) Robotic chemical discovery system driven by convolutional neural network.[102]

(C) Autonomous polymer synthesis in conjunction with the TSEMO multi-objective algorithm.[103]

(D) Chemistry automated by LLMs.[30]

Adapted with permission from (A and D) ref.,[30,101] Springer Nature Ltd.; (B) ref.,[102] ACS; (C) ref.,[103] RSC. IR, infrared spectroscopy; NMR, nuclear magnetic resonance.

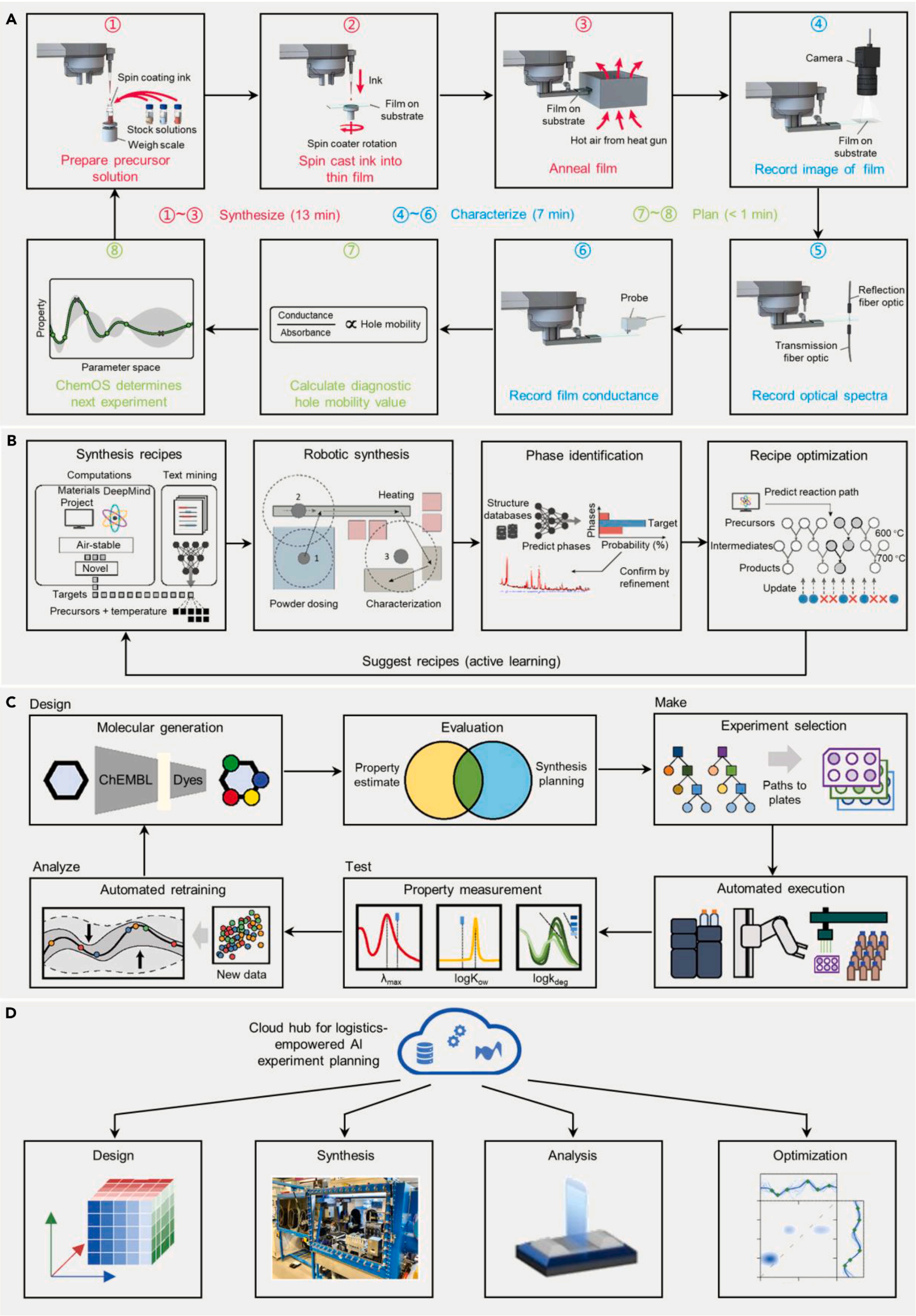

Figure 7. Autonomous workflows for inverse design through potential design-synthesis-manufacturing closed cycles

(A) Iterative design to discover thin-film compositions.[79]
(B) Accelerated synthesis with robots with optimized parameters.[21]
(C) Autonomous molecular discovery through DMTA cycles.[34]
(D) Delocalized, asynchronous, closed-loop discovery of organic laser emitters.[7]
Adapted with permission from (A, B, and D) ref., AAAS; (C) ref.,[21] Springer Nature Ltd.

optimize reaction yields) in low-dimensional spaces but becomes computationally prohibitive for scenarios with more than 20 variables such as in multi-component alloy design.[55] Reinforcement-learning systems like those used for robotic nanofabrication[105] adapt well to parameter drift but require 10–100 times more data than the Bayesian approach, making them impractical for resource-intensive characterization scenarios. Generative models like MatterGen[72] accelerate discovery of novel crystals faster than random sampling by embedding formation energy thresholds into the diffusion process, but their predictions often overlook kinetic barriers for experimental viability. The true power of all these methodologies emerges through their integration: Bayesian optimization guides reinforcement learning's action spaces to avoid costly parameter regions, while generative candidates seed experimental queues pre-screened for scalable synthesis pathways. This synergy creates a robust paradigm for materials discovery that balances performance, cost, and scalability. Such integration is operationalized through model-assisted modular experimental platforms with complementary aspects of autonomous systems: closed-loop optimization,[33] iterative design,[37] self-driving experiments,[79] DMTA cycles,[34] and asynchronous cloud-based delocalized closed-loop (ACDC) discovery.[7] Rather than operating in isolation, these approaches are functionally interdependent, collectively contributing to achieve target-value-oriented products.[7] They serve as foundational tools within the broader architecture of autonomous systems, enhancing both experimental efficiency and decision quality.[30] Alongside model-driven approaches, model-free strategies have also advanced autonomous systems. These data-intensive methodologies rely directly on empirical data, enhancing flexibility and adaptability in unstructured experimental environments.[3]

By combining model-driven inference and model-free exploration, the capabilities of autonomous inverse design have been significantly expanded, allowing for more robust and versatile systems.[21] This expanded capability is further reinforced through the real-time integration of digital twins further strengthening this framework, which facilitates real-time data sharing and simulation as well as optimizing the experimental design even before physical synthesis begins. Additionally, the integration of hardware and software automation systems is equally important, which ensures coherent execution of synthesis parameters across modular automation platforms.[7,21] Key achievements have been achieved across AI algorithms, software function, hardware implementations, experimental scales, performance metrics, and application domains. These findings are summarized in Table S3; this table features data on the inverse designs and the manufacturing of various materials, such as copolymers,[107] thin films,[24,79] photocatalysts,[6,29,37,108] solid inorganic powders,[21] and perovskites.[82]

Advancing from this robust foundation, intelligent algorithms are transforming the understanding of chemical reactivity by extracting insights from nonconvex models,[79] nonlinear interactions,[29] and high-dimensional parameter spaces[80] within closed-loop paradigms. For instance, the reaction selection index (RSI) facilitates automated identification of the most reactive pathways, enabling targeted reaction exploration[101] (Figure 6A). Convolutional neural networks (CNNs) further abstract chemical reactivity from reagent identities, allowing for high-level pattern recognition in complex datasets[102] (Figure 6B). Advanced optimization algorithms such as Thompson sampling efficient multi-objective optimization (TSEMO)[103] (Figure 6C) and q-expected hypervolume improvement (qEHVI)[24] capture intricate interdependencies among reaction variables and optimize reaction conditions with precision.[37] Autonomous agents such as Coscientist[30] (Figure 6D), AutoGen,[109] ChemCrow,[110] and ORGANA[111] exemplify the potential of generative AI, especially LLMs in experimental planning and on-demand synthesis execution.

Building on the algorithmic advances discussed above, recent breakthroughs in autonomous synthesis have further enhanced closed-loop systems, ranging from self-driving closed-loop systems[79] (Figure 7A), autonomous systems using active learning and AI[21] (Figure 7B), DMTA cycles exploring the structure-property relationship[34] (Figure 7C), and ACDC research to drive multiple geographically distributed platforms[7] (Figure 7D). These breakthroughs offer the potential to determine unknown factors or parameters from observed results, enabling (1) the refinement of reaction conditions (e.g. 107 out of 4,500 possible reaction options),[79,108] (2) the optimization of synthesis parameters (e.g. 41 out of 58 target materials that span 33 elements and 41 structural prototypes over 17 days),[21,29] and (3) the discovery of a record-low-threshold organic solid-state laser molecule (<75% amplified spontaneous emission threshold of previous record) with synergy across seven geologically delocalized places and the maximization of product yields (with a yield exceeding 95% for the desired product).[30,34,37] Within these workflows, reading modules powered by AI dynamically interface with doing modules driven by automation, forming self-optimizing systems capable of thinking toward material discovery targets.[18] This evolution redefines the material discovery process from a human-centric trial-and-error approach to an accelerated, hypothesis-driven, machine-augmented paradigm, marking a critical inflection point in the future of embodied intelligence for material intelligence.

Embodied intelligence deeply integrates AI within robotic systems to establish dynamic, closed-loop workflows encompassing simulation, synthesis, and experimental validation cycles.[7,112,113] This integration is enabled through continuous real-time feedback from advanced sensor systems, including *in situ* spectroscopy[6] and neuromorphic phase-detection sensors,[114] which facilitates direct interaction between computational models and experimental hardware. For instance, mobile robotic chemists can adapt their sampling paths based on the real-time crystallinity data.[6] While neuromorphic sensors are capable of detecting phase transitions in intelligent matter substrates, prompting autonomous adjustments to experimental protocols.[114] These capabilities effectively blur the traditional boundary between computation and physical experimentation by enabling AI-driven decisions at a hardware level (e.g., reaction termination or parameter tuning) without human intervention. As critically noted by Messeri and Crockett,[98] such embodied systems are essential to avoid the illusions of understanding that can occur when AI models generate physically implausible hypotheses, ensuring that predictions remain experimentally grounded.

Recent advances in material intelligence demonstrate remarkable progress across the reading-doing-thinking paradigm. In data-guided rational design (reading), interpretable machine-learning models for electrocatalyst development[115] now bridge simulation-experimentation gaps, while generative AI[116] allows the extraction of insights from fragmented data, overcoming the limitations of scarce, high-quality, and labeled datasets. Automation-enabled controllable synthesis (doing) has been transformed by digital twins,[97] which virtualizes robotic platforms to optimize parameters pre-execution, solving reproducibility challenges in high-throughput systems. For autonomy-facilitated inverse design (thinking), the active-learning algorithms have enabled the optimization of biodegradable films,[117] demonstrating how closed-loop systems balance sustainability and performance. This triad of advances, such as robust data assimilation, cyber-physical experimentation, and autonomous optimization, confirms material intelligence as a unified paradigm where computational prediction, robotic validation, and AI-driven iteration co-evolve to transform materials discovery.

In a broader context, the convergence of AI and robotic platforms technologies is driving a transformative shift in materials discovery, enabling intelligent experimental planning and autonomous exploration of experimental spaces. Digital twins provide a virtual platform for real-time feedback, allowing autonomous systems to learn from experimental data, refine conditions, and optimize decision-making before physical trials. By automating the exploration of experimental parameters, AI-powered systems[21] eliminate suboptimal synthesis parameters, accelerating closed-loop workflows for inverse design and materials synthesis.[15,34,37] These autonomous systems can further enable the discovery of eco-friendly materials by iteratively optimizing for sustainability metrics such as biodegradability and energy efficiency, supporting next-generation materials with reduced environmental impact.[12] Such integration not only enhances sustainability, precision, and efficiency but also empowers breakthroughs from pharmaceuticals to advanced manufacturing.[12] Ultimately, the synergy of AI, automation, and digital twins in experimental processes will

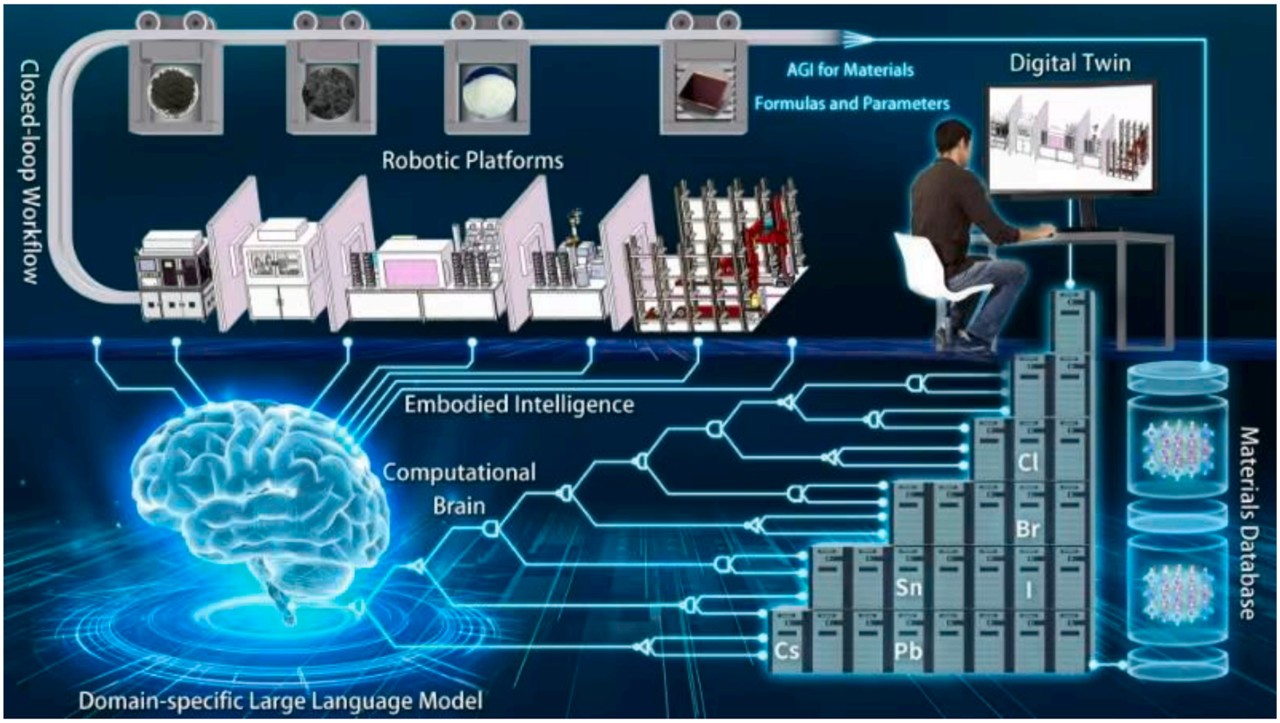

Figure 8. Outlook of material intelligence

reshape the future of materials science, advancing material intelligence toward fully autonomous discovery and innovation.[7,30,48]

CONCLUSION

The emergence of material intelligence, which is an interdisciplinary paradigm that synergizes AI and robotics to emulate and even transcend human cognitive and manual capacities, has begun to redefine the landscape of materials discovery and design. This review articulates a transformative framework unifying three foundational processes in materials research—data-guided rational design (reading), automation-enabled controllable synthesis (doing), and autonomy-facilitated inverse design (thinking)—into a closed-loop paradigm. Recent research has demonstrated significant progress across all three domains. Rational design has benefited from robust databases, informatics tools, and LLMs for knowledge extraction. Automated synthesis platforms offer unprecedented control, precision, and throughput in materials fabrication. Inverse design approach has become increasingly autonomous through the integration of AI agents, generative modeling, and digital twins. These advances collectively redefine how materials are designed, synthesized, and optimized. This increases target-oriented inverse design in experimentation, achieved through the formulation of scientific hypotheses, the protocol of decision-making algorithms, and the closed-loop optimization of materials formulations and parameters. Reading-doing-thinking defined the operating principles of material intelligence as a new era of scientific exploration. The field is poised to enter the next paradigm of scientific discovery characterized by AI conjecture, robotic platform collaboration, and intelligent material experimentation.

OUTLOOK

As material intelligence evolves from task-specific discovery of novel formulas and the optimization of synthesis parameters, it promises to unlock unprecedented precision by AI and robotics, ultimately reshaping the role of scientists as architects of self-evolving material paradigms. Despite the substantial progress made in developing material intelligence, several challenges (Figure 8) remain to be addressed to facilitate its broader adoption and transformative impact across materials science research.

(1) Data standardization for the universal chemistry and materials database. The availability of high-quality standardized data is essential for the success of rational design. However, inconsistencies of data standards and formats, variable quality of data across sources, and the interdependence of multisource data significantly continue to hinder progress. Therefore, establishing unified cross-modal databases that combine multidisciplinary knowledge is imperative. Moreover, automated general strategies allow the rapid identification of reproducible and machine-readable data, further accelerating the development of standardized universal databases. Noteworthy, it is important to establish standardization of instrument output, laying the foundation for consistent data reporting, LLMs and robotics readable data format, material domain-specific knowledge distilling from LLMs, robotics, and even scientists.

(2) Algorithmic innovations for rational design, experimental design, and controllable synthesis. In the realm of automation-enabled materials preparation and synthesis, existing algorithms have underestimated the capacities of automated interactive platforms and the diversity of communication patterns, thereby hindering the development of complex, dynamic, and versatile workflows and experiments. To address this, the development of general-purpose algorithms can effectively diffuse information in literature reviews, synthesis-route planning, and programmable hardware. General-purpose algorithms transform experimental design and controllable synthesis by incorporating new responsibilities, such as prompt engineering and cybersecurity.[18,23] Hence, vertical domains are cultivated by merging domain-specific knowledge with algorithmic innovations to enhance their performance in materials preparation and synthesis.

(3) Enhancing reproducibility and scalability through next-generation robotic platforms with embodied intelligence. Advanced robotic systems have notably improved reproducibility by standardizing synthesis parameters and minimizing human-induced variability. However, challenges such as inconsistent equipment calibration, batch-to-batch reagent variability, and algorithmic discrepancies continue to impact cross-platform

reproducibility. Additionally, the complex processes of atomic rearrangement and microscale crystal growth demand robots with exceptional precision, flexibility, and speed, which are constrained by the high cost of precise manipulation and the complexity of custom setups. Such dependence on specialized robotic platforms limits accessibility, as many laboratories still lack the infrastructure or funding for such systems—a critical gap that demands cost-effective, compact, and user-friendly alternatives. To address these constraints, future innovations must focus on integrating real-time monitoring, digital twin technologies, and standardized calibration protocols. Furthermore, developing modular automated platforms that balance batch synthesis exploratory flexibility with the precision and scalability of flow-based methods offers a promising pathway. These hybrid systems, supported by human-AI-robot collaborative environments, are poised to deliver high-precision, reproducible, adaptive, and scalable synthesis solutions, driving the next generation of intelligent materials manufacturing.

(4) Advancing closed-loop workflows for inverse design. Closed-loop workflows have accelerated multi-objective optimization to satisfy specific formulation or process conditions.[37] However, there are several bottlenecks, including the absence of real-time AI recommendation and evaluation system, lack of interpretable design and adaptable control of robotics, and limited database of structure-property correlations for inverse design. To realize the full potential of inverse design, orchestration of fully autonomous synthesis needs to evolve beyond static feedback cycles. This requires dynamic scheduling, dynamic hypothesis revision, and real-time decision-making powered by domain-specific LLMs and AI agents capable of self-correction and exploration. Bridging this gap also demands interoperable platforms that unify modeling, experimentation, and validation into a coherent paradigm, underpinned by transparent data provenance and standardized metadata schemas. Consequently, such advancements will enable autonomous systems to execute synthesis tasks and to interpret failures, revise assumptions, and discover unknown design principles—marking a shift from automation to scientific reasoning.

(5) Computational brain and scientific hypotheses by autonomous strategies. Although autonomous exploration has been successful for organic molecules, catalysts, nanoparticles, photovoltaics, and batteries, existing algorithms often struggle to efficiently navigate the high-dimensional parameter spaces of molecules and materials for high-performance products. To address this, emerging approaches inspired by the concept of a computational brain aim to emulate human-like reasoning for scientific hypothesis generation and experimental prioritization. Such systems facilitate adaptation to uncertainties in reactants, products, and synthesis parameters, supporting dynamic experiment selection and closed-loop learning. Recent developments in large-scale generative models exemplify this vision: GPT-4 demonstrates strong reasoning ability in text-based scenarios.[30] Kling can generate structured, context-aware visualizations from text instructions,[118] and the Universal Manipulation Interface (UMI) framework unlocks adaptable robot manipulation capabilities.[119] Scaling such intelligent systems in materials synthesis will empower robots not only to execute with precision but also to enable specialized material generation, allowing for the exploration of novel material properties and complex multi-functional designs that are tailored to specific applications. This future will be defined by scalable AI models with versatile robotics conducting highly efficient autonomous unmanned experiments across applications to realize material intelligence.

(6) Reliability, interpretability, and debuggability of artificial general intelligence (AGI) in the context of materials discovery and beyond. The integration of AGI into materials design represents a paradigm shift—enabling the discovery of novel formulas, parameters, reaction mechanisms, and latent physical laws beyond conventional search boundaries. However, this strategy faces fundamental challenges in terms of prediction reliability, insufficient depth of logical deduction, and limited interpretability and debuggability. To ensure its effective use, AGI systems must meet stringent standards for scientific accuracy while maintaining explainable decision-making processes and robust failure-recovery protocols. These requirements become particularly crucial when considering the visionary concept of a universal material code—a standardized, executable framework that can democratize autonomous discovery across distributed labs and even extraterrestrial environments. Such material codes will integrate symbolic AI representations (e.g., chemical programming language like XDL[78]) with structured, FAIR-compliant metadata to encode material formulas, parameters, and structure-property relationships. The implementation of such AGI systems will require overcoming fundamental barriers in scientific accuracy, descriptor standardization, and hardware resilience, alongside addressing ethical concerns around dual-use risks and cybersecurity vulnerabilities. Responsible innovation frameworks must be established to guide AGI development, ensuring that advances in autonomous science align with broader societal and scientific values.

In alignment with the quantitative mission of chemistry and materials science, we are actively responding to this symbol by launching general-purpose technologies capable of processing diverse inputs to generate precise and intelligent outputs. Our goal is to leverage AGI and innovative robotic platforms to empower material intelligence with unique capabilities of synthesis and characterization to broadly address major pain points for large-scale scientific discoveries and scale up materials innovation with embodied intelligence.

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AUTHOR CONTRIBUTIONS

X.Z. wrote the original draft. X.Z., Z.C., F.C., B.F., H.H., and H.Z. reviewed and revised the manuscript. H.Z. conceived the idea and designed the review core framework. H.Z., J.J., H.H., A.A.-G., L.C., and S.Z. supervised the progress of the review. B.W. provided literature support. Z.N. manipulated pictures. J.Y., G.C., J.L., R.L.Z.H., X.L., S.Y.C., W.F., C.-c.C, and C.-y.C. edited the review. All authors discussed the review and commented on the manuscript.

DECLARATION OF INTERESTS

The authors declare no competing interests.

SUPPLEMENTAL INFORMATION

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