

modules with real-time analysis features [90]. A high-precision module mixes multiple reagents, which then flow into a reactor for continuous synthesis. A short-path flow cell enables rapid exploration of quantum dot compositions by measuring photoluminescence at high concentrations without dilution. This system continuously identifies optimal synthesis pathways and saves the key data for scaling up production with minimal starting materials.

In 2024, RoboChem was introduced as a robotic platform to autonomously optimize and enhance photocatalytic reaction processes [91]. Using a graphical interface, users define parameters, while Python-controlled instruments carry out experiments and relay data in real time to a BO framework. This closed-loop methodology reduces the reliance on manual intervention or expert oversight and concomitantly enhances operational safety. The platform efficiently traverses extensive parameter spaces to ascertain optimal conditions for various substrates and augments both reaction yields and space-time yields.

The convergence of autonomous platforms with three-dimensional printing represents a critical trajectory for the field as demonstrated by the Bayesian autonomous experimental researcher (BEAR) developed to navigate the design space of additive manufacturing [92]. BEAR integrates five FDM printers with a six-axis robotic arm and includes a mass balance and universal testing machine to evaluate material toughness. Bespoke orchestration software synchronizes these instruments to execute high-throughput, closed-loop experiments that autonomously optimize metamaterial architectures and processing parameters. The platform rapidly quantifies uncertainty regarding mechanical properties such as toughness and delineates structure-performance relationships which results in a nearly 60-fold reduction in the experimental volume required to identify high-performance designs compared to a grid search. When coupled with topology optimization and analogous design methodologies, the BEAR system elucidates novel avenues for mechanical materials discovery and the identification of previously inaccessible properties.

1.4.3.2 Software Platform

The ARES team proposed in 2018 that autonomous materials discovery could accelerate in a Moore's Law-like manner. By traversing multidimensional parameter spaces with a speed exceeding human capability, these systems effectively manage the high-dimensional intricacies inherent to contemporary materials science [84]. This concept was put into practice in 2021 with the launch of ARES OS, an open-source operating system built to fully manage ARES hardware [84]. The architecture of ARES OS is predicated on three primary modules encompassing interfaces alongside data analysis and design planning. The interface module guarantees fluid interoperability with peripheral hardware and software to ensure precise command execution and data transmission. Concurrently, the data analysis component utilizes sophisticated algorithms to interpret experimental outputs and detect latent patterns or anomalies to drive optimization. The design planning module synthesizes experimental objectives with available resources and analytical feedback to formulate strategic protocols such as the optimization of reaction parameters for carbon nanotube generation. IBM's RXN platform employs a Transformer model with an attention mechanism to automatically learn reaction rules from literature,

enabling the accurate prediction and optimization of both forward and reverse synthesis pathways for target compounds [93].

1.4.3.3 Autonomous Experiments Driven by LLMs

The arrival of LLMs has further accelerated autonomous experimentation, exemplified by the 2023 A-Lab, which leveraged computational modeling, machine learning, and active learning to produce 41 new inorganic compounds in 17 days [94]. This project selected various oxides and phosphates using phase stability predictions, then refined natural language model-proposed syntheses through thermodynamic active learning—a process where analyzing failures yielded practical insights, ultimately demonstrating the high success rate and effectiveness of merging computational science with robotic automation.

Powered by advanced LLMs such as GPT-4 [76], Coscientist autonomously handles the full research cycle, from information gathering and experiment design to code generation and remote laboratory control. Coscientist's software collects publicly available compound data from the Internet and academic sources. After training, it designs a synthesis route and determines the necessary experimental steps, then remotely directs a pipetting robot to carry them out. By using chemical data in SMILES format, the system automatically writes code to enable communication between its modules. Coscientist successfully combines lab automation with LLMs, overcoming traditional experimental barriers and opening new possibilities for autonomous intelligence in chemistry research.

1.4.4 Intelligent Computation

AI-driven materials computation integrates high-throughput computing, multi-scale modeling, and Integrated Computational Materials Engineering (ICME), enabling systems to autonomously guide exploration, method selection, resource allocation, and screening. These autonomous processes operate across the entire material life cycle—from design and preparation to processing and final use—forming a closed feedback loop of virtual tests that generate optimal designs for experimental and engineering applications. Computational intelligence helps overcome the cognitive biases common in traditional human analysis by independently exploring variables outside conventional search areas. Such refinement of technical pathways and design concepts boosts computational efficiency and improves the reliability of materials screening.

1.4.4.1 Machine Learning Interatomic Potentials

Molecular simulations have traditionally been built on empirical potentials informed by experiments or quantum mechanics. However, these methods become significantly less efficient as system complexity increases. Machine-learned interatomic potentials (MLIPs) provide an effective remedy to these computational limitations [95, 96]. These potentials utilize algorithmic learning to automatically derive energy functions from reference data which facilitates the rapid and precise prediction of particle interactions. Relative to standard quantum mechanical techniques, MLIPs provide substantial gains in computational speed and possess the adaptability to

model diverse complex materials by capturing intricate interactions that elude classical descriptions.

Pioneering efforts in this field predominantly utilized artificial neural networks to predict potential energy based on all atomic coordinates within specific systems [97]. While effective in isolated contexts, the reliance of these early models on their training systems severely restricted their broader applicability and accuracy. To surmount these hurdles, deep-learning algorithms have ascended to a dominant position within MLIP architecture. Deep neural networks are capable of decoding complex atomic interactions via nonlinear mappings across multiple neuronal layers and demonstrate superior performance when applied to high-dimensional systems and massive datasets. Furthermore, GNNs enhance MLIPs by learning interatomic relationships directly from graph-structured data.

Deep learning has catalyzed the creation of diverse MLIP frameworks such as the DeePMD-kit developed by DP Technology [98]. By learning the underlying many-body interaction patterns, deep neural networks allow the platform to predict material potential energies with higher accuracy than classical approaches. The integration of molecular modeling, HPC, and machine learning enabled molecular dynamics (MD) simulations of up to 100 million atoms [99–101]. Another important software for large-scale atomic simulations is GPUMD [102]. Integrating GPU acceleration with neural network potentials, GPUMD efficiently models atomic interactions and maintains high accuracy across diverse materials.

1.4.4.2 Efficient Computation and High-throughput Screening

Conventional computational approaches struggle with high-dimensional data, but AI combined with DFT, MD, and high-throughput computation (HTC) is revolutionizing materials screening and analysis.

Machine learning has dramatically sped up DFT, enabling property predictions orders of magnitude faster than conventional approaches [34, 35, 103]. This computational expediency arises from the capacity of these models to assimilate DFT-generated data which subsequently facilitates rapid experimental iteration and process automation. Machine learning algorithms trained on extensive datasets also enhance predictive reliability by mitigating errors and approaching the inherent noise floor of the data which is a critical attribute for compound ranking. By embedding physical principles and refining feature sets, these models effectively navigate data imperfections and improve transferability by internalizing electronic structure information. Deep learning integrated with DFT allows a neural network to represent the Hamiltonian efficiently, bypassing costly self-consistent field calculations while preserving accuracy for twisted van der Waals systems [33]. Furthermore, AI augments the scalability of DFT for macroscopic architectures by generalizing knowledge from localized atomic environments to facilitate the rigorous examination of complex material structures.

Conventional MD simulations often become prohibitively resource intensive as system complexity escalates and result in voluminous datasets that are difficult to interpret. By uncovering hidden patterns in massive simulation logs, AI overcomes limitations of conventional analysis methods [104, 105]. By training models to detect these concealed patterns, automated data processing dramatically increases research productivity. By applying a fully connected neural network

to 180,000 membrane designs, researchers quickly identified optimal candidates based on structure–conductivity correlations [106]. Such predictive capabilities offer precise initialization points for subsequent simulations and obviate the burdensome assumptions inherent in manual trial and error. Additionally, AI is pivotal in optimizing simulation parameters such as time steps and force fields which historically required extensive empirical adjustment. By learning from historical archives, machine learning models can forecast optimal settings based on specific simulation objectives and system characteristics to enhance both the efficiency and fidelity of MD research.

HTC inherently involves massive datasets and complex procedures which frequently leads to the curse of dimensionality when managing high-dimensional variables. Machine learning provides robust support in this arena by employing data-driven methodologies to discern valuable patterns and optimize workflows for materials screening [107]. These algorithms analyze historical records to identify critical variables and recognize previously neglected factors to refine the scientific rationale underpinning material design. When screening materials, models trained on existing datasets can prioritize candidates, filtering promising options from a large pool and offering reliable evaluations early in the design process. DeepMind’s GNoME model, trained on first-principles data, generated 2.2 million crystal structures, with an estimated 380,000 likely stable. This breakthrough expanded the catalog of known stable crystals more than 10-fold and set a new standard for discovery [108].

ALKEMIE (Artificial Learning and Knowledge Enhanced Materials Informatics Engineering), a key development in Materials Genome Engineering, uses its AMDIV framework—automation, modularity, database integration, and visualization—to enable data-driven research. ALKEMIE stores all structured and multimodal data in the Matter Cloud, which offers high-level APIs for easy querying and sharing. The repository currently holds over 600,000 crystal structures, 10,000 phonon spectra, 100,000 DFT band structures, 1,000-GW-accurate band structures, and 200,000 machine learning potential datasets [109]. In a parallel vein, researchers from the Chinese Academy of Sciences engineered the MatCloud platform [110], which utilizes a hybrid quantum mechanics–machine learning strategy to forecast material properties. The ProME platform, as shown in Figure 1.8, tackles materials challenges in extreme environments with a suite of validated proprietary

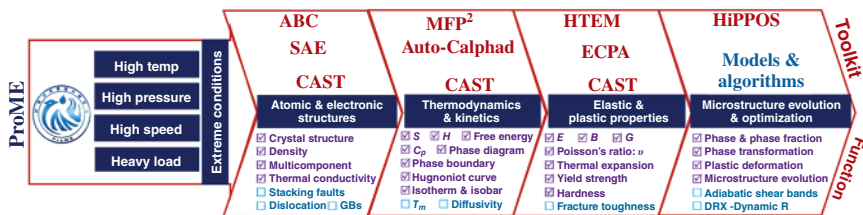


Figure 1.8 Toolkits and their functions within the ProME platform. *Source:* [111] / John Wiley & Sons / CC BY 4.0.

tools—including those for creating ordered and disordered crystal lattices and modeling their properties—centered around a self-adaptive core that manages workflows and corrects errors during HTC [111].

1.4.4.3 AI-enhanced ICME

ICME combines experiments, computational modeling, and engineering design. It uses multi-scale simulations to link atomic and macroscopic processes, optimizing production paths and predicting performance before manufacturing. Key tools include material databases, property-prediction models, microstructural models, and cost analysis [112]. The increasing complexity of materials design presents challenges for traditional ICME in handling high-dimensional, nonlinear problems. AI integration offers a solution by analyzing large datasets to uncover hidden patterns, optimize parameters, and complement physical models, thereby enhancing accuracy, efficiency, and progress in the field.

AI coupled with ICME now leverages extensive datasets to clarify microstructure–property links, enabling more precise materials predictions [113]. Where explicit physical models are incomplete or unavailable, AI provides distinctive advantages. AI-enhanced ICME in multi-scale modeling combines cross-scale data integration with automated parameter tuning to improve predictive accuracy and robustness [114, 115]. This capability is especially important for high-performance and application-specific materials.

The combined use of AI and ICME has delivered concrete progress. Researchers established composition to processing to structure to property relationships for cemented carbides using a multi-loop machine learning framework, enabling intelligent design [116]. Data-driven ICME was also used to design lightweight and high-entropy alloys [117]. Integrating phase-field modeling with deep VAEs enables microstructure design and accurate thermal conductivity predictions [118]. These examples show the strength of combining machine learning, knowledge-based modeling, and established ICME systems.

AI-assisted design and manufacturing are now core, data-intensive elements of the ICME era [112, 117]. As shown in Figure 1.9, the smart materials paradigm is shifting from knowledge- and data-driven ICME toward an AI⁺ era—moving from “designing materials” to “designing with materials” [111, 112, 117]. This progression advances from Embedding AI through Copilot AI toward emerging AI Agent systems [111].

While the MGI focuses on experiments, computation, and databases, Human–Cyber–Physics and Materials Genome Engineering frameworks center on human–machine interaction [119]. Their intersection points toward future advanced-AI applications. Machine learning can speed up fundamental science by revealing key data relationships, strengthening Human–Cyber–Physics interpretation and leading to new principles [120]. Industry 4.0, driven by data and AI, extends digital integration through cyber–physical systems, now giving rise to Materials 4.0 [121]. Figure 1.9 compares top-down engineering and bottom-up computational design [122].



Figure 1.9 The field is moving beyond data-driven ICME, entering an AI⁺ era of intelligent materials design and manufacturing [112, 117]. Inset of the Materials Innovation Platform adapted from [129].

DTs enable real-time, information-physical integration and are key enablers for smart manufacturing in aerospace, rail, and engine sectors [111, 117, 123]. Process-to-structure and structure-to-property models underscore how materials knowledge turns data into manufacturing intelligence [122, 123]. With advances in LLMs and next-generation AI [124–126], human–cyber interaction will evolve significantly, continuing the shift from material design paradigms toward designing with materials in the AI⁺ era [127, 128].

1.4.5 Intelligent Manufacture

1.4.5.1 AI-assisted Additive Manufacturing

Subtractive manufacturing can be inefficient and costly for complex components. Additive manufacturing, or 3D printing, circumvents these limitations by fabricating intricate parts directly from digital designs, streamlining production and reducing material and time costs. Selective laser melting produces precise parts like the C919’s winglet bar and NASA’s fuel nozzle with minimal scrap [130], while also enabling novel materials such as NASA’s GRX-810 alloy [131] and China’s adaptable mechanical metamaterials [132, 133].

Advances in materials, technology, and AI have rapidly expanded the potential of 3D printing, enabling its use with metal [134], polymer [135], ceramic [136], composite [137], and biological materials [138] to transform digital manufacturing. AI transforms every step of the process—from choosing material compositions [139]

and designing structures [133] to optimizing the printing process [140]. It analyzes large datasets to propose new material formulas, designs stronger and lighter shapes, and adjusts printing settings in real time to improve precision and reduce errors [141]. These innovations make 3D printing more adaptable, sustainable, and precise, advancing smart manufacturing.

1.4.5.2 AI-integrated DT

DT is an effective tool to bridge the physical and digital worlds in smart manufacturing, using continuous data synchronization to strengthen decision-making, enable predictive adjustments, and support autonomous optimization. For instance, researchers developed a Hall–Petch model guided by decision trees that, using key parameters like grain boundary energy and valence electron distance, allowed metallic properties to be optimized in real time without empirical fitting [67]. DT methods have refined laser powder bed fusion for Inconel 718 and accelerated homogenization, and when combined with CNNs, they improve creep fracture life predictions in titanium alloys [142, 143]. In smart manufacturing, researchers developed a deep-learning-integrated DT for real-time defect control in hot-rolled coils [144] and a separate DT model using real-time vibration and temperature data to predict CNC machine tool failures [145].

1.4.5.3 AI Agent-driven Material Manufacturing

LLMs' rapid progress is advancing automation toward smart manufacturing through the rise of intelligent agents [146]. An agent is an intelligent system that perceives its environment, makes decisions, and executes tasks. It learns, adapts, and collaborates, continuously interacting with its surroundings and adjusting through feedback to form a closed-loop process [147].

Agents enhance smart manufacturing at every level. Locally, they improve process optimization, quality control, and equipment management. They replace slow, error-prone manual checks with fast, consistent, and data-driven automated inspections. By integrating AI with vision and sensor technologies, manufacturing systems can detect defects, anticipate equipment wear, and dynamically adjust processes for customized outputs [148, 149].

Though still emerging in smart manufacturing, agents are already showing strong benefits in materials research [146]. For instance, the Material Intelligence Scientist System, developed by the Shanghai Institute of Ceramics, integrates autonomous learning, data extraction, and lab interaction to efficiently optimize materials. The platform autonomously generated a lithium-rich cathode with 282 mAh/g capacity and 100% retention after 20 cycles, surpassing previously reported performance.

Figure 1.10 shows an LLM-driven workflow for optimizing microstructure and classifying defects in welded titanium alloys [111, 150]. It integrates automated coding, image processing, and machine learning to analyze high-throughput welding images, improving defect detection efficiency and reliability. This demonstrates the potential of AI agents to advance smart manufacturing through enhanced process control and innovation.

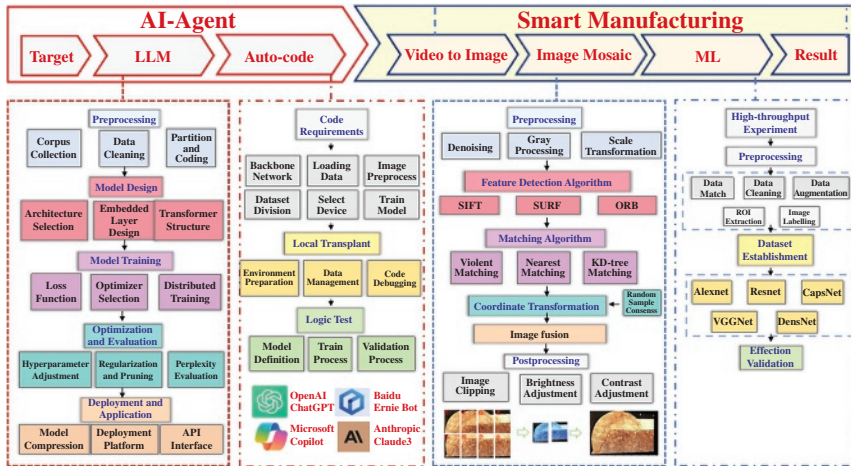


Figure 1.10 An LLM-driven workflow for optimizing microstructure and classifying defects in welded titanium alloys. *Source:* [150] / OAE Publishing Inc. / CC BY 4.0.

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