

Large Language Models in Nanoparticles Research: Methods, Applications, Impacts, and Future Directions

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Abstract: Large Language Models (LLMs) have emerged as a cutting-edge tool in the era of advanced science and technology, in materials science by enabling novel approaches such as the development of open-source libraries, intelligent research tools, AI accelerated design platforms, AI driven morphology prediction and related innovations. By 2026, a remarkable transition is evident from experimental adoption of artificial intelligence towards its large-scale integration across diverse industries driven by LLMs to understand complex tasks and execute with high accuracy. This review underscores the potential of LLMs in the advancement of nanomaterial and nanoparticle research and positioning them as an alternative-approaches to conventional computational and experimental methods. This study also analyzes and summarizes procedure of LLM-based methodologies in nanomaterial research like automated knowledge extraction, Retrieval-Augmented Generation (RAG), domain specific fine tuning, hypothesis generation and synthesis planning, knowledge graph construction, LLM based agents and research workflows. Moreover, the implementation of LLMs across various domains, such as environmental sustainability, drug delivery systems, health surveillance, biomaterials, and tissue engineering, is discussed in this literature review, which also proposes future research directions to guide further advancements in this rapidly evolving field.

Keywords: large language models (LLMs); artificial intelligence (AI), machine learning

1. Introduction

The innovation and development of emerging nanomaterials with requisite features are critical for resolving global obstacles in numerous domains, for instance health surveillance, energy, environmental sustainability, etc [1]. However, traditional trial-and-error methods for material synthesis are time-consuming, domain-specific, and constrained by the inherent complexity of material construction [2]. Acceleration of this process because of the ongoing demand of the development of new material and the advancement of new technologies is very crucial at this moment. Despite the Machine Learning (ML) arisen as a high-performance tool in the case of elevating discovery of material and optimization [3,4], the obstacles of acquiring a robust dataset for the training of ML models remains the same. This data deficiency acts as a major roadblock to the implementation of ML for prediction and optimization in various areas, requiring an alternative approach to data generation and model training. The modern-day structural design of Large Language Model (LLM) represents the pinnacle of a multi-



decadal evaluation, advancing from 1950s symbolic logic and stochastic foundations to emerging high-dimensional neural attention mechanisms. A seminal information-theoretic frameworks by Shannon (1948, 1950), utilize mathematics to test the efficiency of simple models to speculate or compress text [5]. Subsequently these models become pioneer of various features, including recognizing speech, translating languages, and searching for information. The recent cutting edged Large Language Models (LLMs) established via transformer-based architecture, optimized through large scale pre-trained data from the publicly accessible repositories, has resulted a significant advancement in algorithmic efficiency across divers domains. Lately, LLMs have become the cornerstone technology for developing basic artificial intelligence (AI), serving as foundational frameworks for simulating human- level high-order cognitive computation. LLMs have entered the mainstream due to their excellent language comprehension and generative capabilities. These AI models are engineered to parse, interpret, and generate coherent natural language. Upon analyzing the structure and underlying logic of the data, they developed a new word sequence that flows naturally from the input. In recent years, these models have begun integration into diverse areas of science beyond traditional language tasks [6]. Moreover, contemporarily, the rapid advancement of LLMS has gained significant scholarly interest. Several studies provide structured overviews based on development stages including pre-training, fine-tuning, evaluation, and application while also tracing the evolution of language models and key technologies [7].

AI and ML has made possible to analyze large collections of materials data to find hidden patterns, predict material properties, and support experimental design. Rapid advancements in computing power and the volume of data generated by automated experiments and high-speed simulations have propelled this progress. Building on these advances, LLMs go beyond traditional ML methods by using information from unstructured text sources, providing a broader and more powerful approach for data-driven discoveries in materials science and technology [8].

The formidable capabilities inherent in Large Language Models (LLMs), as known Figure 1, originate from three foundational architectural components within the Transformer framework. To facilitate the models to prioritization of pivotal words in a sentence and their comprehension of word relationships, even when they are far apart, Transformers first employ a self-attention mechanism. Second, Transformers can process many parts of the data simultaneously, which makes training and computation much faster. Lastly, the Transformer design adheres to the scaling hypothesis, meaning that a model's performance significantly improves with an increase in size, training data, and computing power [9].

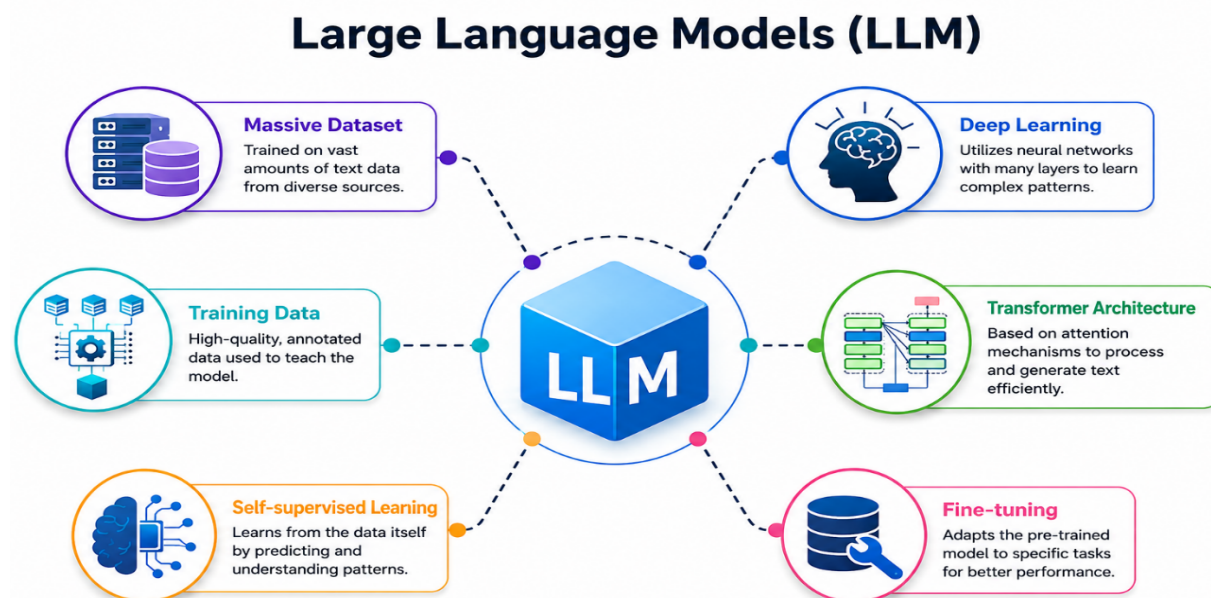


Figure 1. Large Language Model.

Data-driven generative modeling techniques have emerged as state-of-the-art mechanisms for material design. During this process, target properties—such as mechanical, thermal, or optical characteristics—are defined, and appropriate compositions and techniques are chosen to attain them. Transformers, diffusion models, generative adversarial networks (GANs), and variational autoencoders (VAEs) are important generative frameworks. In particular, VAE-based models, learn compact data representations and generate new material structure, aiding the optimization of nanomaterial design [10].

LLMs founded upon decoder-only transformers aid nanoparticle research through knowledge discovery and data-driven insights [6]. LLMs are capable of facilitating nanoparticle research by analyzing vast amounts of scientific literature, discovering and designing new nanoparticles, interpreting experimental data, and predicting their future properties. Furthermore, these models can generate ideas and descriptions to assist with new experiments and applications [11]. The manipulation and engineering of materials at the nanoscale, usually between 1 and 100 nanometers is none as nanotechnology. The combination of various materials, instruments and systems results in materials with distinct physical and chemical characteristics at this scale [8].

LLMs are excellent at text mining, summarization [12], and information extraction, as they are based on the Transformer architecture and trained on vast corpora of scientific literature. These skills are highly valuable in catalysis research, where extracting insights from disparate literature is essential for identifying synthetic pathways, evaluating performance metrics, and predicting catalyst properties. Their ability to produce structured outputs, like JSON or tables, enables them to be essential for developing comprehensive systems that convert raw research papers into machine-readable data for analysis. Utilizing LLMs to analyze scientific papers is still a work in progress, however, it demonstrates significant advancement in fields such as nanomedicine. This capability enables the automation of collecting structured and organized information regarding nanoparticle design from research papers, which minimizes the manual effort typically required [13].

Nanoscience has advanced swiftly in recent years, resulting in significant research on nanoparticles-materials with unique physical and chemical properties at the nanoscale. Despite this advancement, the vast amount of unstructured writing in this field creates a barrier to collecting and analyzing information efficiently. Traditional manual methods are time consuming and frequently lack consistency, driving a need for intelligent automation in data extraction and knowledge organization.

Recent developments in LLMs, which are advanced neural architectures trained on extensive text corpora, have transformed the paradigm of processing and understanding information [14]. LLMs have shown great promise in material science beyond normal language tasks. For example, these models are capable of automating literature mining, synthesis extraction, and property prediction (Figure 2) [15]. Their capacity to interpret and summarize complex scientific texts can speed up the process of discovery and enhance research efficiency.

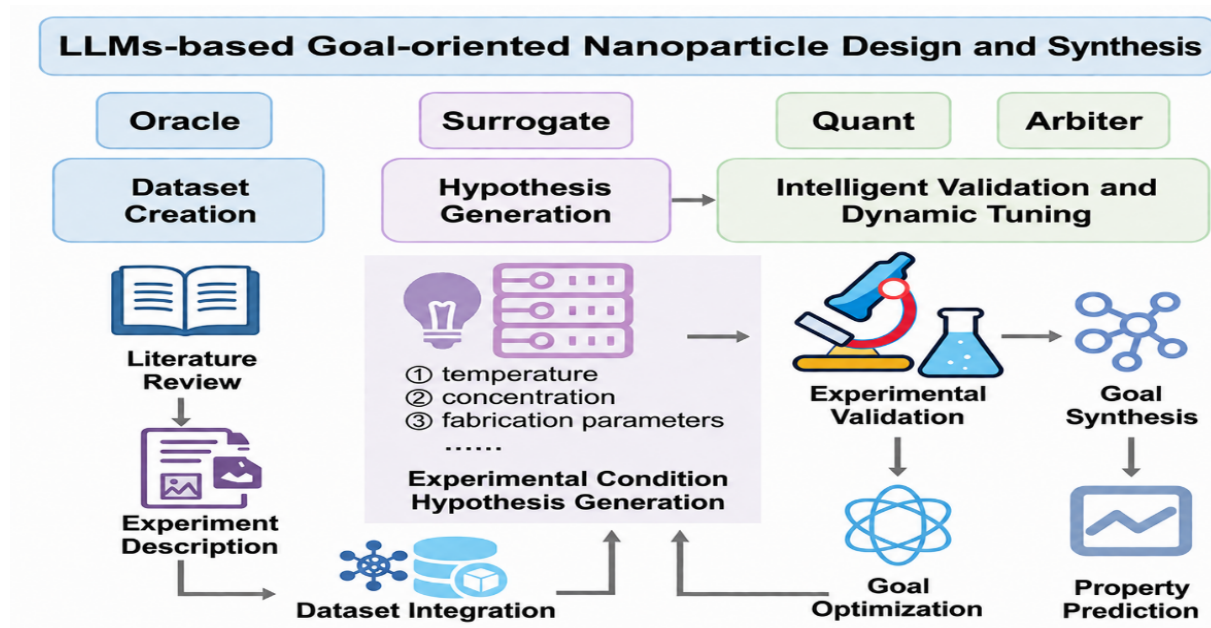


Figure 2. LLMs-based Goal-oriented Nanoparticle Design and Synthesis.

This paper explores how LLMs can be applied to nanoparticle research, particularly in automating literature analysis, data extraction, and hypothesis generation. Despite the progress in AI-assisted materials research, the systematic integration of LLMs into nanoparticle studies remains limited. Therefore, this review paper aims to highlight both the potential and challenges of combining Natural Language Processing with nanoscience.

2. Overview of Large Language Models (LLMs)

Large Language Models (LLMs) represent a major breakthrough in natural language processing (NLP), driven primarily by advances in Transformer architectures, large scale pre-training and task specific adaptation

strategies. Their ability to learn rich linguistic representations from massive unlabeled corpora has made them powerful tools across scientific domains including nanomaterials and nanoparticles research. This section provides overview of the core components of LLM development: (i) pre-trained language models, (ii) model pre-training, (iii) fine-tuning and downstream adaption and improved and emerging LLM techniques.

2.1. Pre-trained Language Models

Pre-trained language models form the backbone of modern NLP systems. PLMs fundamental purpose is to capture general linguistic and semantic patterns from large amounts of unlabeled texts, enabling them to transfer effectively to downstream scientific or industrial tasks. Early representation models such as word2vec [11] and Glove [16] introduced static word embeddings but they were limited in contextual understanding. The breakthrough came with contextualized models like ELMo [10] and the Transformer architecture [17]. These two are used in bidirectional LSTMs to generate dynamic word representations and self-attention, enabling parallelization. This architecture serves as the foundation for nearly all modern LLMs.

Modern PLMs are now categorized into three primary types. Encoder-only models such as BERT [18], RoBERTa [19] and DeBERTa [20] provide strong bidirectional representations for text comprehension, making them suitable for classification and extraction applications. Decoder model such as GPT-2 [21], GPT-4 [22] and LLaMA [23] are designed for next-token prediction giving them powerful generative and reasoning functions. Lastly encoder-decoder, sequence-to-sequence models including T5 [24] and FLAN-T5 [25], integrate various NLP tasks by employing a text-to-text paradigm. Pre-trained LLMs can perform well on new and unseen tasks. However, since they are mainly trained to predict the next word or token, they may struggle to fully understand use intent and can sometime produce harmful, biased or incorrect responses [26]. In nanoparticle research, these PLMs facilitate the extraction of synthesis parameters, the parsing of microscopy data, the identification of nanoparticle characteristics, and the organization of unstructured scientific information into formats amenable to computational analysis.

2.2. Model Pre-Training

Pre-training is the foundational phase in which a LLM learns broad, general-purpose language representations by processing massive collections of unlabeled text from a variety of sources, including books, articles, web pages, and scientific corpora. This stage is very important because it gives to learn basic language patterns, semantic relationships, and how to understand things in context before it has to do any specific tasks. In most real word domains especially scientific or technical fields high quality labeled datasets are limited, costly to create and unevenly distributed across tasks. LLMs build a strong universal language base during pre-training by using large-scale unsupervised or self-supervised learning. LLMs develop a strong universal language foundation that can later be adapted to small, domain-specific datasets through fine-tuning or prompt-based methods. In the Figure 3 flow diagram illustrate the main stage of pre-training development. Prompting can occur at different points in the process, such as after pre-training or instruction-tuning or alignment tuning. In the diagram, ‘RL’ refers to reinforcement learning, ‘RM’ to reward modeling and ‘RLHF’ to reinforcement learning with human feedback.

LLMs learn general-purpose and linguistic and world knowledge from billions of tokens using self-supervised objectives. Masked language modeling used in BERT and RoBERTa, trains models to reconstruct randomly masked words, enabling rich bidirectional context learning [15,16]. Autoregressive language modeling used in the GPT family [18,19], trains models to predict the next token in sequence, producing fluent generation. Span corruption, introduced with T5 [24], masks entire spans of text and requires to regenerate them, improving long-range dependency handling. Pre-training draws on large, heterogenous datasets like web pages, books, scientific articles and scaling laws [27] demonstrated that model performance increases predictably with more parameters, more data and more compute. This understanding enabled models with hundreds of billions of parameters, though recent work highlights the importance of data quality rather than sheer scale alone. For scientific disciplines such as nanoscience, pre-training equips LLMs with foundational linguistic and conceptual understanding of chemistry, materials terminology, structure-property relationships and experimental conventions, making them immediately useful even before specialized fine-tuning (Figure 4).

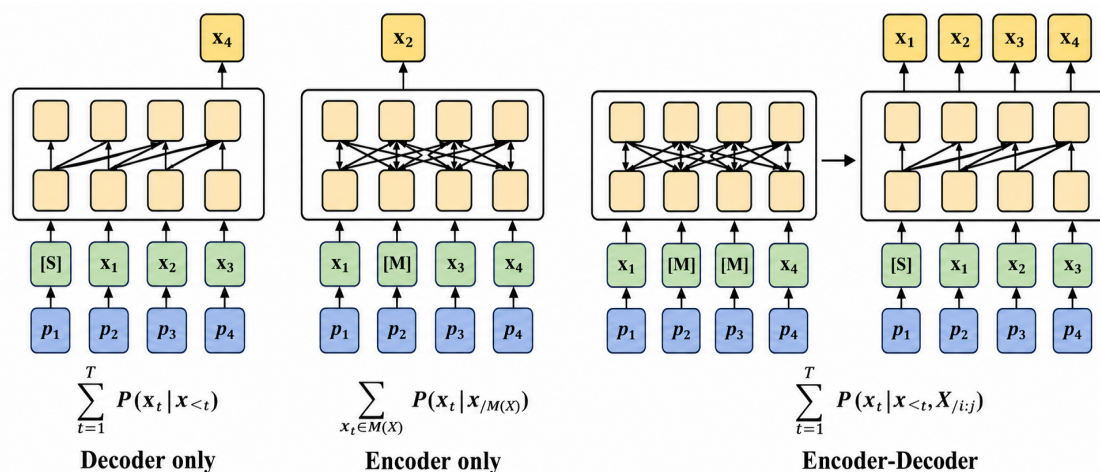


Figure 3. An illustration of the commonly used pre-training frameworks [15].

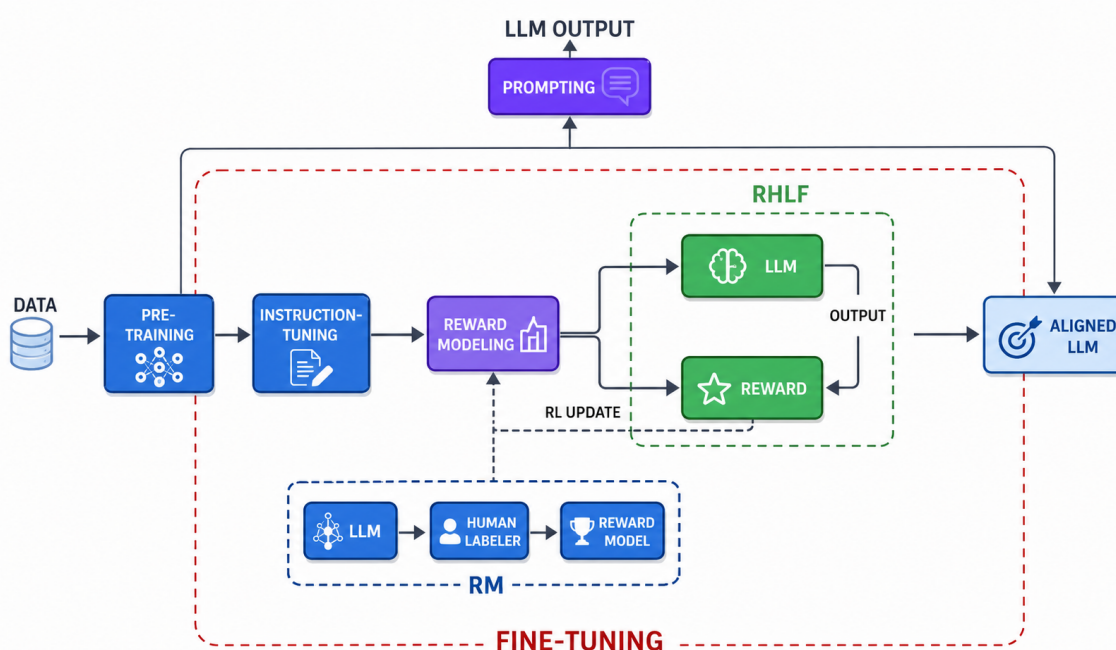


Figure 4. A simple flow diagram showing the main stages of LLM development from pre-training to real-word use [26].

2.3. Fine-Tuning and Downstream Adaptation

The process of fine-tuning (Figure 5) involves applying a large pre-trained model on a smaller, task-specific dataset. The objective is to help the model in modifying its general knowledge so that it can function effectively on a specific domain or application. Full fine-tuning was the original type of fine-tuning. This method uses labeled examples from the target task to update all of the model's parameters on labeled task data [18]. Full fine-tuning entails retraining each and every part of a pre-trained model with hundreds of millions or even billions of parameters. Although this method usually gives strong performance.

Fine-tuning and other downstream adaption techniques are necessary to successfully deploy LLMs for particular scientific tasks. Moderns LLMs often rely on instructions through curated datasets such as FLAN [25], dramatically improving their controllability and generalization. Reinforcement learning from Human Feedback (RLHF) first widely applied in InstructGPT [28] and later in GPT-4 [22], aligns model outputs with human preferences by optimizing them against a reward model trained on human judgments. To reduce resource requirements, parameter-efficient fine-tuning (PEFT) techniques modify only small portions of the model. Methods such as Adapters [29], LoRA [30] and prompt or prefix tuning [31] allow domain specialization with minimal computation and without overriding the base model's general knowledge. For nanoparticle-focused tasks, these methods enable the creation of compact, domain-specific models capable of extracting synthesis parameters,

classifying nanoparticle morphology, processing SEM/TEM descriptions, and summarizing complex experimental workflows, all without requiring laboratory-scale computational infrastructure.

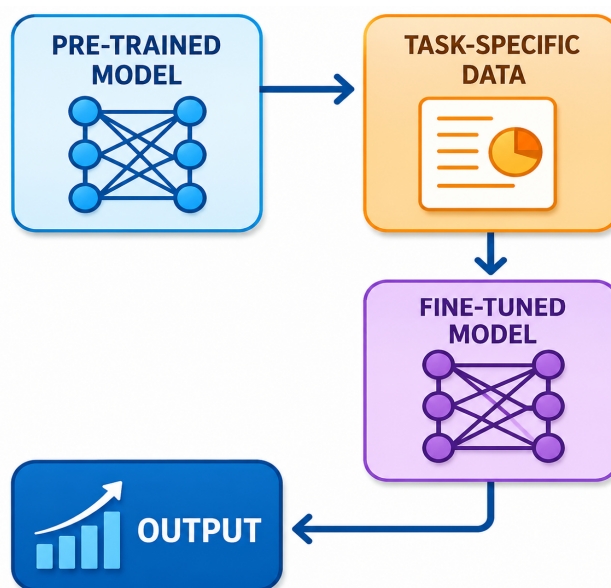


Figure 5. Flow diagram that shows how fine-tuning works.

2.4. Improved and Emerging LLM Techniques

LLM development is further accelerated by several emerging techniques aimed at improving model efficiency, accuracy and scientific reliability. Mixture-of-experts (MoE) models such as GLaM [32] activate only a small subset of expert networks for each input, allowing extremely large effective model capacity while keeping computational cost manageable. Retrieval-augmented generation (RAG) [33] integrates external knowledge sources, like scientific databases, materials repositories or nanoparticle handbooks directly into the generation process, reducing hallucination and improving factual grounding. Compression and distillation techniques, including quantization, pruning and knowledge distillation (e.g., DistilBERT [34]), enable deployment on resource-limited devices making LLMs more accessible for laboratory automation or real-time analysis. Another transformative direction is multimodal LLMs such as GPT-4V and LLaVA [35] which jointly process visual and textual information. These models can interpret microscopy images, associates morphological features with textual descriptions, and bridge the gap between visual nanoparticle characterization and written scientific reporting. Alongside these advancements the evaluation of LLMs through broad benchmarks including SuperGLUE [36], MMLU [37] and HumanEval [38] remains crucial. Although scientific domains increasingly require specialized evaluation metrics tailored to factual accuracy, reproducibility and experimental reliability. Ensuring safety, mitigating hallucinations and improving robustness are recognized challenges as LLMs becomes deeply integrated into scientific research workflows.

3. LLMs Methods in Nanoparticles Research

The use of LLMs in nanoparticles research is growing quickly. Different methods, demonstrated in Figure 6, are being explored to take advantage of what these methods can do well. Most of these methods fall into a few clear groups collecting and organizing existing knowledge, using that knowledge to predict material properties, creating new ideas or experimental plan and combining information from many scientific studies.

3.1. Automated Knowledge Extraction from Scientific Literature

Automated knowledge extraction is one of the most mature and impactful applications of LLMs in nanoparticle research. Scientific publications in nanotechnology are largely written in unstructured natural language making large-scale data reuse challenging. LLMs address this limitation by identifying and extracting key experimental variables such as precursor materials, synthesis conditions, nanoparticle size distributions, morphologies, surface modifications and measured properties directly from text. This enables the transformation of dispersed qualitative into machine-readable datasets. Compared to traditional rule-based text mining, LLM-based extraction captures contextual dependencies and implicit scientific relationships, which are common in

nanoparticle synthesis descriptions. As a result, these systems significantly accelerate literature analysis and enable systematic mapping of synthesis-structure-property relationships across vast research corpora [39,40].

3.2. Retrieval-Augmented Generation (RAG)

Retrieval-Augmented Generation enhances LLM reliability by grounding generated outputs in external scientific evidence. In nanoparticle research, where precision and reproducibility and critical, RAG systems retrieve relevant journal articles, reviews or database entries and provide them as contextual input to the model during response generation. This approach allows LLMs to generate explanations, summaries or comparisons that are explicitly supported by existing literature. RAG frameworks are particularly effective for answering targeted questions related to synthesis optimization, comparative performance of nanoparticles or interpretations of experimental trends. By reducing reliance on internal model memory alone, RAG methods improve factual accuracy and transparency, which are essential for scientific writing and decision making [7,41].

3.3. Domain-Specific Fine-Tuning of LLMs

Fine-tuning LLMs on nanoscience and material-specific datasets further improves their suitability for nanoparticle research tasks. During fine-tuning, model parameters are adjusted using curated corpora containing experimental reports, synthesis protocols and material databases. This process allows the model to internalize domain-specific terminology, experimental logic and casual relationship commonly encountered in nanoparticle research. Fine-tuned model shows enhanced performance in recognizing materials entities, understanding synthesis workflows and interpreting characterization results. Such specialization is particularly important when dealing with complex chemical nomenclature or nuanced experimental descriptions that general purpose may misinterpret [42].

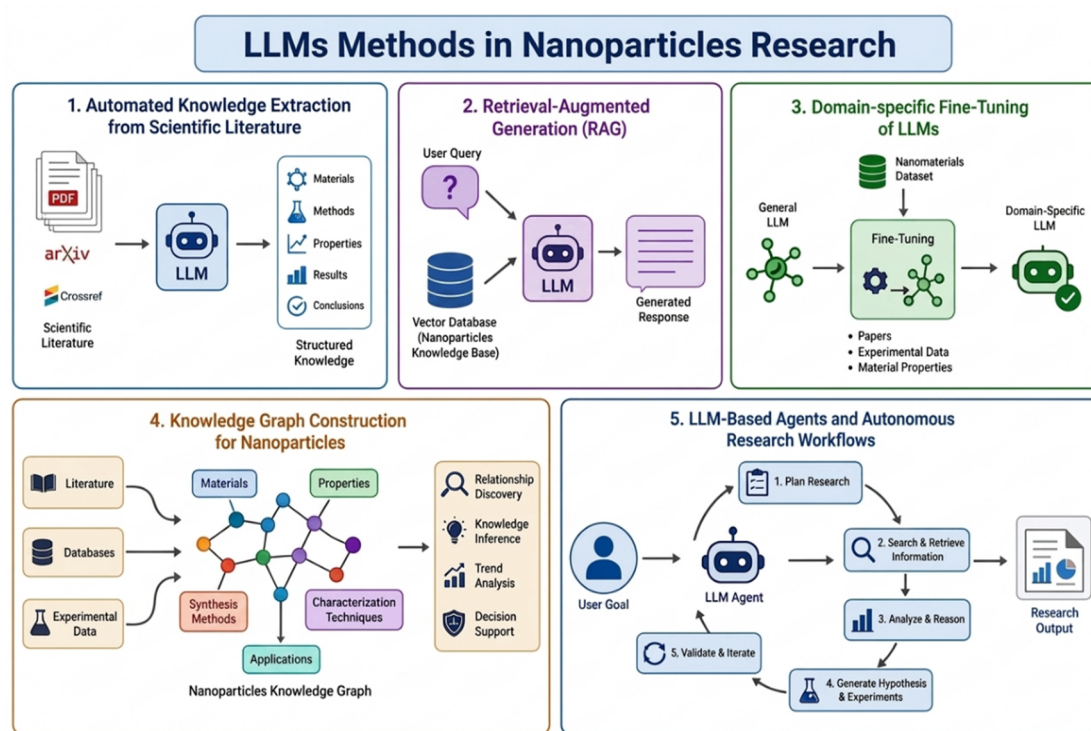


Figure 6. LLM methods in Nanoparticle research.

LLMs are increasingly used as cognitive tools to assist hypothesis generations in nanoparticle research. By synthesizing patterns across existing studies, LLMs can propose potential synthesis strategies, parameter variations or mechanistic explanations for observed nanoparticle behaviors. This method is especially valuable interact in non-linear ways. While the generated hypotheses require expert validation and experimental verification, LLM-assisted ideation can reduce exploratory effort and highlight promising research directions. Recent studies demonstrate that LLMs can reason beyond surface-level pattern matching and provide chemically meaningful insights when appropriately prompted.

3.4. Knowledge graph Construction for Nanoparticles

Knowledge graph [43] construction represents a structured extension of LKLM-based extraction methods. In this approach, extracted information is organized into graph-based representations where nodes correspond to entities such as materials, synthesis methods or properties and edge represent their relationship. Knowledge graphs enable complex querying, visualization of interdependencies and integration with predictive machine learning models. In nanoparticle research, these graphs facilitate exploration of supporting data-driven discovery. LLMs play a critical role by enabling scalable extraction and semantic alignment of entities before graph construction [7].

3.5. LLM-Based Agents and Autonomous Research Workflows

LLMs are increasingly integrated into agent-based systems that coordinate multiple research tasks autonomously. These agents combine language understanding with access to tools such as scientific databases, simulation platforms or laboratory automation systems. In nanoparticle research, LLM-based agents can iteratively analyze literature, propose experiments, interpret results and refine hypotheses. This approach supports closed-loop research workflows that reduce manual intervention and accelerate discovery cycles. Although still an emerging paradigm, early demonstrations suggest that LLM-driven agents may play a significant role in future autonomous nanomaterials research environments [8,44].

4. Application of LLMs in Nanoparticles

Nanoparticles engineered structures with dimensions on the order of 1–100 nanometers occupy a central role in modern science due to their unique physical, chemical and biological properties. Nanoparticle research also generates an enormous amount of experimental and computational data, much of which is reported in unstructured text across thousands of scientific articles. Managing, interpreting and reusing this information efficiently remains a major challenge. In recent years, LLMs have emerged as powerful tools capable of addressing this challenge. Since 2021, there has been rapid growth in applying LLMs in increasing attention on nanoparticle-related research domains. The integration of these technologies creates new opportunities for sustainable innovation and human-centered applications, illustrated in Figure 7.

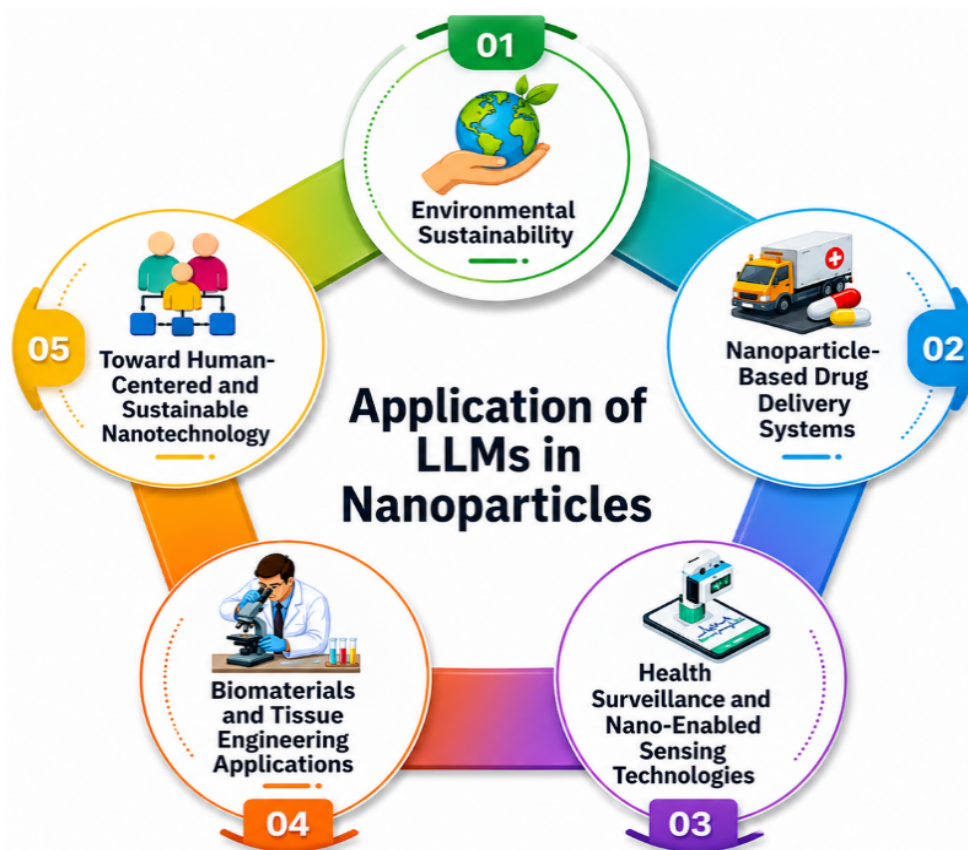


Figure 7. Applications for LLM in Nanoparticles.

4.1. Environmental Sustainability

Environmental sustainability is one of the most critical global challenges and nanoparticle-based technologies play a significant role in addressing pollution, energy efficiency and resource management. Nanoparticles are widely used in water purification, pollutant degradation, carbon capture and renewable energy systems due to their high reactivity and tunable surface properties. However, designing environmentally efficient nanomaterials requires understanding complex interactions between material composition, environmental conditions and long-term stability. LLMs contribute to sustainability-focused nanoparticle research by analyzing large environment and materials datasets, extracting insights from dispersed literature and identifying environmentally friendly synthesis pathways. Recent studies show that AI models including LLM-assisted workflows help optimize nanomaterials for reduced toxicity lower energy consumption during synthesis and improved lifecycle performance [45].

4.2. Nanoparticle-Based Drug Delivery Systems

Nanoparticle-based drug delivery systems (NDDS) have become an important strategy for improving drug stability, bioavailability and therapeutic efficiency. Nanoparticles typically range from 1–100 nm allowing them to encapsulate drug and release them in a controlled manner while reducing systemic toxicity [46]. Their large surface area and tunable surface chemistry enable efficient drug loading and functionalization for biomedical applications [47].

Nanoparticles are widely recognized as powerful carriers for targeted drug delivery, offering controlled release, improved bioavailability and reduce side effects. Designing effective nanocarriers requires balancing multiple factors including particle size, surface functionalization, drug loading efficiency and biological compatibility. The literature in this area is vast and rapidly growing. LLMs help address this complexity by systematically analyzing biomedical literature, clinical trial reports and preclinical studies related to nanoparticle drug delivery. A key advantage of NDDS is targeted drug delivery. Nanoparticles can accumulate in diseased tissues through the enhanced permeability and retention effect, which occurs due to the leaky vasculature of tumors. This property improves drug concentration at the target site while minimizing damage healthy tissues.

4.3. Health Surveillance and Nano-Enabled Sensing Technologies

Health surveillance systems increasingly rely on nanoscale sensors and diagnostic platforms for early disease detection, environmental monitoring and public health management. Nanoparticles enhance biosensor sensitivity by enabling selective molecular recognition and signal amplification. These nano-enabled devices generate large streams of heterogeneous data including sensor readings, patient records and environmental measurements. LLMs play a critical role in transforming this raw data into actionable knowledge. By processing clinical notes, sensor metadata and scientific guidelines, LLMs can support real-time health surveillance, anomaly detection and assessment [48]. Recent studies demonstrate that AI-powered language models enhance the interpretation of biosensor outputs and facilitate communication between technical systems and healthcare professionals.

4.4. Biomaterials and Tissue Engineering Applications

Biomaterials and tissue engineering play a crucial role in regenerative medicine by providing materials that support the repair or replacement of damaged tissues. Biomaterials such as hydrogels, polymers and nanomaterials are commonly used because they can mimic the structure of the extracellular matrix and promote cell adhesion, proliferation and differentiation [49]. Nanoparticles are essential components in biomaterials and tissue engineering, where they improve mechanical strength, bioactivity, and cellular interactions. Applications include bone scaffolds, wound healing materials, and implant coatings. Designing biomaterials with optimal biological performance requires integrating knowledge from materials science, biology, and clinical research.

Recently LLMs and natural language processing techniques have been used to support research in biomaterials and tissue engineering. LLM-based systems can analyze large collection of biomedical publications to extract information about biomaterial compositions, fabrications methods and biological responses. This automated knowledge extraction helps researchers identify promising materials, compare experimental outcomes and accelerate the design of advanced biomaterials for regenerative medicine applications [39,43].

4.5. Toward Human-Centered and Sustainable Nanotechnology

The integration of LLMs with nanoparticle research aligns with a broader shift toward human-centered, sustainable, and data-driven science. Rather than replacing experimental work, LLMs act as intelligent collaborators that enhance human reasoning, reduce redundant experimentation, and promote responsible

innovation. Recent perspectives argue that AI-assisted nanotechnology can significantly reduce development time while supporting ethical and environmental considerations [39,50].

5. Related Work Analysis

The Large Language Model is cutting edge technology which has the potential to build advanced technology which can lead us to the future, to solve the unsolved mystery, to build a personalized artificial mate for different professionals. A lot of researchers have done their work on this particular topic and bring advancements in different aspects. In this portion we discuss the work which we have done in the previous several years, also illustrated these in Figure 8.



Figure 8. Previous LLM Research.

5.1. Nanoparticle Synthesis, Design, and Morphology Control

The research described in [51] aims to explore the use of ML to predict the morphology of Copper Nanoparticles synthesized via the microwave-assisted polyol method. To achieve this, the researchers developed small, carefully curated datasets from only 25 in-house syntheses. This model can effectively make quantitative predictions about the Cu NP synthesis results.

A comprehensive set of 775 multiple-choice questions was developed in investigation [52], focusing on LLMs' capabilities regarding the synthesis mechanism for assessment in the field of gold nanoparticles (AuNP). The results illustrate that the combined use of confidence scores (c-scores) and the benchmark successfully distinguishes between LLM responses based on a mechanistic physicochemical understanding and those that are random.

The potential of artificial intelligence to predict the shape and size of nanoparticles using a recently compiled collection of diverse data formats for calcium carbonate nanoparticles was highlighted in [53]. This compilation contains various types of shapes within one particular chemical system. By training and optimizing a tree based ensembled model to predict multiple categories of nanomaterial morphologies, researchers subsequently investigated the capabilities of LLM on the same task. The LLM demonstrates superior performance in small data scenarios. The final outcome was a text-to-image prototype capable of predicting nanoparticle images directly from synthesis parameters.

Study [54] introduced a collaborative framework, which utilizes a hybrid approach combining search-based algorithms with a fine-tuned Llama-2 Large Language Model (LLM). Developed by compiling and analyzing 492

seed-mediated AuNP synthesis protocols from online literature sources, the study established that the type of seed capping agent plays a vital role in determining the morphology of the AuNP.

For the development of a comprehensive dataset of seed-mediated Gold Nanoparticle (AuNP) synthesis recipes aimed at understanding synthesis control, scientists [55] proposed a hybrid approach combining search-based algorithms and a Large Language Model (LLM). This dataset demonstrates two key findings: first, that the choice of seed capping agent influences the final morphology of the AuNPs, and second, that there is a correlation between the aspect ratio of the final Gold Nanorods (AuNRs) and the concentration of silver nitrate.

A human-AI collaborative agent introduced in [56] was designed to surmount the bottlenecks of iterative ligand refinement. By leveraging a dataset of harvested literature and merging it with an autonomous pipeline of synthesis, spectroscopy, and computation, the system accelerates the discovery process. The LLM harmonizes distinct elements of the design phase, standardizing them for immediate laboratory implementation in coordination with domain specialists.

To attain meticulous control over the particle size distribution (PSD) of titanium oxide nanoparticles optimized for integration into photonic nanocomposite systems, a GBDT-RR (Gradient Boosted Decision Tree-Rosin-Rammer) framework was developed in [57], utilizing a Bayesian Optimization (BO) algorithmic combination. This platform demonstrates remarkable superiority over established methodologies in empirical trials.

5.2. Biomedical Nanotechnology and Nanomedicine

Researchers developed a data workflow automation in [58], harnessing open-weight Large Language Models (LLMs), which includes an automated process to extract structured nanoparticle-design data from research findings, with a specific focus on blood-brain barrier (BBB) formulations. This system offers a clear demonstration of the potential to systematize a task typically performed by domain experts.

NanoSafari, a generative AI tool that automatically extracts information from publications, was established in [59]. To elevate the reliability of the Large Language Model (LLM), this study developed a dataset with correct and relevant data to serve as an index (or validation set). NanoSafari outperformed the baseline model by providing more reliable parameters for nanomaterial design tasks, as verified by a blinded evaluation conducted by nanoscientists.

In study [60], scientists generated a machine learning workflow using open-source machine learning libraries and microfluidics to create a nanomedicine product. Named MicrofluidicML, this model not only provides a computationally lightweight and researcher-controlled framework, but also complete governance and control over the input data.

Expanding upon earlier approaches [61], developed a non-canonical machine learning model for the virtual screening and optimization of Lipid Nanoparticles (LNPs), the primary delivery vehicle for mRNA vaccines. The methodology harnesses a Large Language Model (LLM) to decisively elevate the prediction of pivotal LNP properties, thereby accelerating the advancement of medicinal innovation. This model delineates higher-fidelity inferences of lipid characteristics compared to established benchmarking methods.

Furthermore, researchers in [62] developed an AI-based automated data extraction pipeline deployed via the Python-based LangChain framework. The primary objective of this study was to enable knowledge extraction from scientific literature and subsequently utilize the data to construct benchmark-setting nanotoxicity prediction models. The AI-based model efficiently collects high-fidelity data, leading to superior predictive accuracy and demonstrating prognosticated utility in the field of nanotoxicity research.

5.3. Advanced Functional Materials (Energy, Frameworks & Photonics)

Investigation [63] developed a nano photonic device based on a large language model. The motive of this project was to signify the capability of LLMs to accelerate the nanophotonic design development and increase its accessibility. This model enhances two key applications by incorporating LLM: multilayer films and optima meta surfaces. For multilayer films, this model improves context learning and facilitates discussion among LLM and users for better results. It also calculates optical responses via simulation and makes progress in optimal designs for user provided target optimal properties. In the terms of optimal meta surfaces, the LLM finetuned it by text-based representation of meta surface structure and properties to generate designs with target properties by adjusting the input and output text. The final results show that the transmission and reflection of multilayer devices can be accurately predicted, even with using few shots Chain-of-thought prompting in domain specific scenarios. Crucially, the model also demonstrates that it can be successful without requiring prior knowledge from the user or database. Moreover, in context learning capability of LLM is extended to inverse design through iterative conversational prompting, resulting in optimal multi-layer film designs for specific optical specification.

Scientists introduced a complete information rich framework designed by Perovskite Solar Cell (PSCs) in [64], to accelerate innovation and discovery in research. The PSCs has three essential parts: Perovskite-KG(a specialized knowledge graph containing 1517 research papers with 23,789 entities and 22,272 relationships),two auxiliary datasets: Perovskite Chat(including 55,101 high-quality query-respond sets developed by a new innovative system involving multiple agents) and Perovskite Reasoning (having 2217 selected, high-quality problems in materials science), two dedicated large language models: Perovskite Chat LLM (designed to provide expert support within a specific area of expertise) and Perovskite-Reasoning-LLM (applied to activities focused on scientific inquiry). The PSCs system illustrates considerably greater effectiveness against existing tools and proves itself as a better knowledge-based assistant in research work.

To elevate molecular search and molecular engineering for enhancing the durability of black phosphorus (BP), researchers in [65] established a data-centric and expertise-based approach combining LLM-based literature analysis, DFT calculations, GNN prediction, and experimental validation. During the test period, the Black Phosphorus stabilized through molecular passivation displayed outstanding passivation effects, demonstrating durability for over 20 days under normal room conditions—a significantly longer period than that observed for unmodified BP.

In the same way, to facilitate material development for researchers lacking specialized computational knowledge, study [66] introduced MOFsyn Agent, an AI-driven framework that employs Large Language Models (LLMs) to accept natural language inputs. This system suggested an innovative sequential reduction strategy, which achieved better results than the traditional one-pot reduction method.

In Study [67], scientists introduce a unified architecture amalgamating scholarly extracted empirical records, accelerated structural assembly, and a multi-objective GNN–DKL architecture. The primary objective of this study is to expand the configuration of organic spacer cations for 2D halide perovskites (HPs) and surmount the hurdles of data-sparse chemical regimes and fragmented bibliographic data. This model demonstrates outstanding performance regarding physicochemical robustness and a low propensity for factual fabrication in comparison to contemporary LLM architectures.

For ease of comparison, the representative studies discussed in this section are summarized in Table 1.

To refine scientific insights into the architecture of Electrode–Electrolyte Interphases (EEIs), researchers in [68] integrate AI-orchestrated, data-driven discovery workflows. This iterative-adaptive model unifies high-throughput experimentation (HTE) and high-throughput computation (HTC) to navigate the “ontology-concept-computation-experiment” continuum. By mitigating the disconnection between nanoscale interfacial dynamics and cell-level operational efficacy, this method fast-tracks material invention and eliminates cognitive bias.

Investigators introduced a closed-loop digital materials ecosystem in [69] that merges data sources, high-throughput experimentation (HTE), universal machine learning interatomic potentials (MLIPs), and Large Language Models (LLMs). This model aims to demonstrate the potential of AI methodologies to transition from manual experimentation to a self-directed research infrastructure. Furthermore, this innovation overcomes the limitations of traditional trial-and-error approaches by utilizing an advanced architecture to simultaneously anticipate material behavior and maximize reaction efficiency.

Table 1. Illustrate that the nanoparticles application papers based LLM model.

Category	Proposed Model	Ref	Year	Architecture	Aim	Strength	Limitation
1. Nanoparticle Synthesis, Design, and Morphology Control	Classical ensemble regression ML	[51]	2024–2025	Input prompt/text → LLM → Code generation or metasurface geometry prediction	To predict the scale of Copper Nanoparticles (Cu NPs) synthesized through microwave-assisted polyol method	Reduces manual design effort; supports code generation; efficient fine-tuning with LoRA	Depends on prompt quality; limited physics reasoning; evaluated on limited device types; text-only representation; limited benchmarking
	LLM	[52]		Benchmark questions → LLM (+ RAG) → Mechanism explanation → Confidence score (c-score)	To analyze the capability for synthesizing logical process rather than unorganized results, specifically in Gold Nanoparticle (AuNP) synthesis	Improved explanation accuracy using RAG; confidence-based evaluation	Limited to Au nanoparticles; relies on retrieved knowledge; evaluates reasoning rather than material design
	LLM	[53]	2024	Synthesis parameters → Feature extraction → ML/LLM model → Morphology prediction (shape/size) → Text-to-image generation	To discover the capability of AI to forecast the morphology of nanoparticles and model a text to image system based on the outcome	Compares ML and LLMs, supports multimodal prediction, enables AI-assisted morphology visualization	Small dataset, limited generalization, low-quality image generation, requires larger multimodal datasets
	Llama-2 LLM	[54]	2025	Scientific literature → Text mining & Llama-2 extraction → Structured synthesis dataset → ML analysis of morphology	To assemble and evaluate a huge number of seed-mediated Gold Nanoparticle (AuNP) synthesis protocols from digitally available literature sources to improve understanding and reproducibility	Creates a large structured dataset (492 validated recipes), automates literature mining, identifies key synthesis factors affecting nanoparticle morphology	Limited to seed-mediated Au nanoparticle synthesis; incomplete or missing information in literature affects extraction; LLM may hallucinate missing recipe details; recipe representation is simplified and lacks complete process information.
	Llama-2 LLM	[55]	2024	Literature → Search parser → Fine-tuned Llama-2 → Structured dataset → Data analysis	To generate a comprehensive data set of Gold Nanoparticle (AuNP) synthesis recipes to gaining clarity to control morphology and size	Combines rule-based parsing with LLMs; constructs a validated dataset of 492 recipes; identifies key synthesis factors (e.g., CTAB/citrate) affecting AuNP morphology; improves reproducibility through structured data extraction.	Limited to seed-mediated AuNP synthesis; extraction quality depends on literature completeness; manual validation is still required; weak correlations for some synthesis parameters; not directly applicable to other nanomaterial systems
	LLM	[56]	2025	Human–LLM dialogue → Ligand hypothesis generation → High-throughput experiments → DFT validation → Morphology optimization	To surmount the inefficiency of conventional experimentation in nanocrystal ligand design by iteratively refining ligand design and speeding the invention of structure-property relationships	Integrates LLM reasoning with experimental validation and DFT; reduces trial-and-error; discovers ligand design principles and facet-specific binding mechanisms	Demonstrated only for CsPbBr ₃ perovskite nanocrystals; relies on expert-guided prompts and experimental verification; LLM predictions are not independently validated without DFT/experiments; generalizability to other material systems remains unproven.
	GBDT-RR (Gradient Boosted Decision Tree-Rosin-Rammler)	[57]	2025	Literature + experiments → LLM-assisted data extraction → GBDT-RR model → Bayesian optimization → Optimal synthesis conditions	To get precise control over the particle size distribution (PSD) of titanium oxide nanoparticles (NPs) for use in optical nanocomposites	Fast inverse design, experimentally validated, transferable to other oxides	Dataset-dependent, requires experiments, limited validation scope
2. Biomedical Nanotechnology and Nanomedicine	Open-weight LLM	[58]	2024–2025	Scientific papers → OCR/XML preprocessing → LLM extraction → JSON output → Judge model refinement	To mechanical nanoparticle design data extraction from academic publications, especially on blood-brain barrier (BBB) formulations	High schema accuracy, automates literature mining, supports structured database creation	Sensitive to PDF/OCR quality, requires human verification, limited to BBB nanoparticle literature

Table 1. Cont.

Category	Proposed Model	Ref	Year	Architecture	Aim	Strength	Limitation
2. Biomedical Nanotechnology and Nanomedicine	NanoSafari	[59]	2025	Literature → GIVE extraction → Nanoparticle database → LLM copilot	To mechanical data extraction from the biomedical nanoscience literature, and supplying correct, trustworthy scientific references and nanomaterial design parameter for biomaterial and bioengineering applications	Reduces hallucinations, extracts data from >20,000 papers, experimentally validated	Depends on extracted database quality, focused on biomedical nanomaterials, requires database updates for new research.
	MicrofluidicML	[60]	2025	Experimental database → ML training → Property prediction → Formulation optimization	To derive a process utilizing publicly accessible machine learning libraries to directing the nanomedicines developments by microfluidics	Accurate prediction, inverse formulation design, experimentally validated	Accurate prediction, inverse formulation design, experimentally validated
	LLM	[61]	2024	Lipid SMILES → Molecular embeddings → CatBoost classifier → Transfection efficiency prediction	To triumphing over the information deficit through the examination of open-access data and applying five diverse molecular description techniques to enhance the prediction and design of Lipid Nanoparticle (LNP) efficacy (TE).	Learns effective molecular representations, improves prediction accuracy, supports virtual screening	Small benchmark dataset, focused only on ionizable lipids, limited generalizability to other nanoparticle systems.
	AI-Driven Automated Pipeline	[62]	2025	Literature → LLM data extraction → Nanotoxicity database → ML prediction	To simplified efficient data collection from publications utilizing an AI based pipeline and then leverage the refined data to develop highly accurate models for forecasting nanotoxicity.	Automates literature mining, improves prediction accuracy, reduces manual data curation	Extraction depends on literature quality, requires validation, limited dataset diversity, performance may not generalize across all nanomaterials.
3. Advanced Functional Materials (Energy, Frameworks & Photonics)	LLM	[63]	2025	Transformer → Prompt Engineering (ICL) or LoRA Fine-Tuning → Photonic Design Output	To analyze the ability to indicate nanophotonic design problems in the absence of specialized knowledge	Reduces manual design effort; supports code generation; efficient fine-tuning with LoRA	Depends on prompt quality; limited physics reasoning; evaluated on limited device types; text-only representation; limited benchmarking
	Perovskite-KG	[64]	2025	Perovskite knowledge base → RAG → LLM → Research assistance and prediction	To establish efficient knowledge management and reasoning system in PSC research to accelerate innovation and discovery	Domain-specific knowledge, reduced hallucination, improved scientific reasoning	Limited to perovskite domain, depends on knowledge base quality, requires continuous database updates, lacks extensive experimental validation
	LLM	[65]	2025	LLM → GNN screening → DFT → Experimental validation	To expedite molecular discovery and leading molecular engineering for improving the stability of black phosphorus (BP)	Screens large molecular space, experimentally validated, improves BP stability	Focused only on black phosphorus, depends on DFT and experiments, limited generalizability.
	MOFsyn	[66]	2025	Material knowledge → LLM candidate generation → ML screening → DFT validation → Experimental verification	To triumph over the inherent limitations of conventional experimentation in Metal-Organic Frameworks (MOF) synthesis and supply a productive tool for intelligent material synthesis	Accelerates molecule discovery, integrates AI with DFT and experiments, experimentally validated	Focused only on black phosphorus, relies on DFT and experimental validation, limited generalizability to other materials system
	combining literature-mined experimental data, high-throughput molecular graph construction, and multitask GNN-DKL modeling (Graph Neural Network with Deep Kernel Learning)	[67]	2025	Literature → RAG extraction → Molecular graphs → GNN-GP → Candidate screening	To speed up the sketch of organic spacer cations for 2D halide perovskite (HPs) and resolve difficulties arising from unknown chemical areas and unreliable published data	Integrates LLMs with GNNs, uncertainty-aware prediction, supports candidate screening	Limited to 2D halide perovskites, depends on literature quality, requires experimental validation, preprint study
	AI-driven big data framework	[68]	2025	Data → AI/LLM → Interphase optimization	Optimize battery interphases	Data-driven design, faster discovery	Data-dependent, requires experimental validation
	AI-assisted catalyst design framework	[69]	2025	Data → ML/LLM → Catalyst design → Experimental validation	Accelerate catalyst discovery and synthesis	Faster discovery, reduces experiments, supports inverse design	Data-dependent, requires experimental validation, limited generalizability

Table 1. Cont.

Category	Proposed Model	Ref	Year	Architecture	Aim	Strength	Limitation
4. Molecular Discovery and Property Prediction	MolRAG (Molecular Retrieval-Augmented Generation)	[70]	2025	Query molecule → Similar molecule retrieval → CoT reasoning → Property prediction	To upgrade LLM performance on molecular property speculation by incorporating Retrieval-Augmented Generation (RAG) with Chain-of-Thought (CoT) reasoning.	Improves prediction accuracy, provides interpretable reasoning, no additional training required	Depends on retrieval quality, limited by knowledge base coverage, evaluated on benchmark datasets only.
	LLM-Struct-Fusion	[71]	2025	Molecular structure → LLM knowledge extraction → GNN fusion → Property prediction	To improve molecular representation of MPP, thereby delivering a dependable and successful remedy that combining broad expert knowledge (LLM) with precise molecular structure-function data.	Enhances GNN performance with LLM knowledge, improves prediction accuracy, captures chemical semantics	Depends on LLM knowledge quality, computationally intensive, evaluated mainly on benchmark datasets, limited experimental validation.
	Retrieval-Augmented Generation	[72]	2025	Scientific literature + laboratory data → RAG → LLM → Nanomaterial design recommendations	To boost up drafting and assessment of nanostructured materials by self-extracting, synthesizing, and providing necessary technical knowledge from broad range of publication	Integrates literature with laboratory knowledge, reduces hallucinations, improves design reliability	Depends on knowledge base quality, requires continuous database updates, limited experimental validation, evaluated on selected nanomaterial systems only.
5. Benchmarking, Knowledge Management & Scientific AI Frameworks	LLM	[73]	2024	Nano synthesis benchmark → LLM (+ RAG) → Mechanism explanation and reasoning	To thorough evaluation of LLMs role to scientific endeavor, specifically to check if their success is based on understanding how the mechanisms work or just on recollecting specific data points	Introduces a 775-question benchmark, proposes the c-score metric, improves reasoning assessment, reduces hallucinations with RAG	Limited to Au nanoparticle synthesis, depends on retrieval quality, benchmark-based evaluation, lacks experimental validation
	NANOGPT	[74]	2025	User query → RAG retrieval → LLM → Nanotechnology-specific responses	To support the nice requirements of nanotechnology research to accelerating learning and idea formulation	Domain-specific retrieval, reduces hallucinations, improves answer accuracy, supports literature exploration	Depends on knowledge base quality, requires regular database updates, limited experimental validation, focused on information retrieval rather than materials discovery
	Spherical LLM-105	[75]	2025		1.preclude the agglomeration of LLM-105 particles during long term preservation 2.optimize reliable system activation while using in a slapper detonator	Combines simulation with experiments; analyzes micro/nano structure effects	Specific to LLM-105 explosive material; no AI/ML methods; limited to initiation performance analysis
	EvoPat	[76]	2024	Patent documents → Multiple LLM agents → Summarization and patent analysis	To efficiently summarize, evaluate, and contextualize patents for professionals and providing comprehensive point of view on content documentation, clarifies groundbreaking ideas	Improves summarization quality, supports efficient patent analysis, reduces manual effort	Depends on LLM performance, limited evaluation on patent datasets, requires high-quality patent documents
	LLM-Feynman	[77]		Scientific data → LLM reasoning → Symbolic regression → Formula discovery	To develop simple and high utility equations from data by incorporating deep domain knowledge by achieving true generalization	Discovers interpretable formulas, enhances scientific reasoning, applicable across scientific domains	Depends on data quality, computationally intensive, benchmark-based evaluation, limited real-world experimental validation
	Learning Advance	[78]	2025	Robotic experiments → GPR + BO → LLM hypothesis generation → Experimental validation	To speed up the invention of chemical knowledge by allowing major discoveries beyond conventional optimization limits by the incorporation of optimization and AI driven hypothesis generation	Integrates robotics, ML, and LLMs; enables closed-loop discovery; experimentally validated	Demonstrated on a specific chemical system, requires robotic infrastructure, computationally intensive, limited generalizability
	VIRSCI (Virtual Scientists)	[79]	2025	Research topic → Multi-agent discussion → Idea generation → Novelty assessment → Abstract generation	To replicate the cooperative approaches to generate new scientific findings and yielding fresh, varied conclusions grounded in realistic team science	Mimics real scientific teamwork, improves idea novelty, supports collaborative reasoning	Depends on LLM and retrieval quality, computationally expensive, lacks experimental validation in real scientific discovery tasks.
	MaScQA	[80]	2025	MaScQA benchmark → LLM → Question answering → Performance evaluation	To set up the baseline performance of existing LLMs (15 different models) on Question Answering (Q&A) tasks in materials science.	Comprehensive benchmark, compares 15 LLMs, establishes baseline for domain-specific LLMs	Limited to QA tasks, no experimental validation, open-source models underperform, lacks domain-specific fine-tuning

Table 1. Cont.

Category	Proposed Model	Ref	Year	Architecture	Aim	Strength	Limitation
6. Scientific Agents, Foundation Models and Autonomous Laboratories	LLM-enabled porous materials research framework	[81]	2026	Text mining → LLM adaptation (Prompt/Fine-tuning/RAG) → Multi-agent systems → Autonomous laboratory	Accelerate porous materials discovery and synthesis using LLMs	Comprehensive review, integrates text mining, RAG, multimodal LLMs, and self-driving labs; outlines future research directions	Review paper (no novel model); relies on existing studies; autonomous laboratories remain immature; challenges include hallucinations, data quality, safety, and high computational cost.
	AutoLabs (Cognitive Multi-Agent System)	[82]	2026	User → Supervisor Agent → Specialized Agents → Self-correction → Robotic execution	Automate chemical experimentation in self-driving laboratories	Multi-agent collaboration, self-correction, >85% error reduction, near-expert performance (F1 > 0.89)	Evaluated mainly on one robotic platform (Big Kahuna), requires LLM reasoning models and laboratory hardware, limited cross-platform validation.
	MOFReasoner (domain-specific reasoning LLM)	[83]	2026	Knowledge distillation + CoT → Fine-tuned LLM → MOF reasoning & prediction	Enhance scientific reasoning for MOF adsorption and materials discovery	Domain-specific reasoning, outperforms GPT-4.5/DeepSeek-R1, DFT-comparable predictions, interpretable CoT	Limited to MOF adsorption, text-only (no multimodal data), requires domain-specific training data
	LLEMA (LLM-guided Evolution for Materials Discovery)	[84]	2026	LLM → Evolutionary search → Surrogate predictor → Memory refinement → Multi-objective optimization	Discover materials satisfying multiple property objectives	Multi-objective optimization, chemistry-informed search, memory-guided refinement, outperforms LLM-only baselines on 14 benchmark tasks	Depends on surrogate model accuracy, requires iterative optimization, evaluated mainly on benchmark tasks (limited experimental validation)

5.4. Molecular Discovery and Property Prediction

To improve LLM efficiency in molecular property prediction, [70] introduces a Retrieval-Augmented Generation framework termed MolRAG. This architecture incorporates retrieval-based augmentation by distilling domain-specific information and integrating it with Chain-of-Thought (CoT) reasoning as a foundational step. Consequently, MolRAG amplifies interpretability in physicochemical attribute inference by offering scholars transparent explanatory frameworks.

Study [71] seamlessly integrates conceptual data from LLMs with molecular motifs derived from structural models to develop a resilient and high-fidelity framework for molecular property prediction. By fusing LLM-derived vectors with topological features, the study creates a hybridized construct that outperforms several pre-trained structural models. Furthermore, this model demonstrates clear superiority over traditional benchmarks across the entire evaluation phase.

5.5. Benchmarking, Knowledge Management & Scientific AI Frameworks

In order to expedite the composition and assessment for nanostructured materials through the automated retrieval, amalgamation, and reporting regarding scholarly data across prolific research archives, researchers developed an AI-driven platform in Study [72]. This platform amalgamates a Retrieval-Augmented Large Language Model (RAG-LLM) with the field-specific datasets. The proposed model not only successfully mitigates factual inaccuracies but also provides empirically grounded responses anchored in referenced literature, representing a substantial upgrade over the inherent rigidity of isolated LLM training data.

775 multiple choice questions associated with the synthesis methods and morphological structure of gold nanoparticles were developed in [73]. This effort aimed to highlight the capabilities of the LLMs in material science and demonstrate their significance in scientific applications and power to reason systematically. Researchers apply knowledge extraction methods and confidence score (c-score) to assess a mix of popular commercial and community-driven LLMs. The results show that the c-scores are superior at distinguishing LLM understanding from mere memorization in synthesis tasks.

Investigation [74] developed NANOGPT, a Large Language Model Retrieval-Augmented Generation (LLM-RAG) system designed as an intelligent research assistant for nanotechnology. LLaMA3.1-8B-Instruct model is incorporated into NANOGPT for its reliable creation and accurate instruction execution capabilities, which boosts effectiveness by accelerating knowledge acquisition and hypothesis formulation during literature review. This model utilizes obtainment using semantic matching, combined with precise optimization, displaying its capability by offering highly relevant and correct conclusions, in terms of researching complex nanotechnology queries. NANOGPT also illustrates its capability for time reduction while maintaining high accuracy throughout its testing period, which showcases this AI-powered tool's ability to revolutionize the querying of scientific literature.

Researchers introduced Spherical LLM-105 in [75], which showcases a micro-nano structure effectively combined using the oil-in-oil emulsion method. Assessment of the surface morphology, crystal structure, thermal decomposition performance, safety performance and short-pulse initiation performance revealed that the new model exhibits improved morphology and an enlarged characteristic drop height, which results in enhanced safety and inhibit agglomeration for prolonged storage. It also demonstrates a decreased short-pulse initiation voltage and exhibits outstanding initiation performance and increased reliability in the slapper detonator.

EvoPat, a multi-LLM-based patent agent designed to assist users in analyzing patents via Retrieval-Augmented Generation (RAG) and sophisticated search techniques, was presented in [76]. This system combines information from various internal sources, such as patents, academic literature, product catalogs, and company-specific data repositories. It also performs real-time online searches to ensure the insights provided are current. EvoPat was evaluated against GPT-4 and sets a high standard in the natural language processing (NLP) domain through rigorous testing.

Study [77] developed the LLM-Feynman framework, an innovative model that leverages Large Language Models (LLMs) with organized optimization for brief results, deriving understandable equations based on observed data and specialized expertise. This model incorporated data preprocessing automation, predictive modeling based on LLM that incorporates self-assessment enhanced by multi-objective optimization techniques and formula explanation by Monte Carlo tree search. This model demonstrates superior performance compared to established techniques (e.g., SISSO, PySR) in the terms of both accuracy and formula complexity, and also displays reliability by successfully deriving the vast majority (90%) of 120 key physical formulas from Feynman's physics collection. This result remains the same in the 2D material synthesizability and perovskites and successfully reached a high degree of correlation ($R^2 > 0.8$) in the estimation of iconic conductivity and GW bandgaps.

Investigation [78] establishes the 'Learning Advance' method, which implements automated field data retrieval by incorporating symbolic information processing within an LLM. The primary objective of this research is to uncover novel chemical insights and optimize chemical systems by emulating traditional human research protocols. This stepwise process successfully reproduces conventional procedures, demonstrating that those possessing minimal domain expertise can unlock new chemical principles using this model.

Researchers engineered a unified architecture named VIRSCI (Virtual Scientists) in study [79] to expedite the research cycle by constructing a framework that mimics the synergistic dynamics of professional scientific inquiry. VIRSCI deploys an ensemble of expert-level agents integrating three core modules: automated idea generation, critical evaluation, and iterative refinement. The proposed model demonstrates a significant inclination toward high-fidelity idea formulation, manifesting unprecedented originality relative to contemporary architectures.

MaScQA, a benchmark designed to institute a performance standard for 15 prevailing LLM frameworks in context-dependent question-answering (Q&A) tasks associated with material science and metallurgical engineering, was proposed in [80]. The MaScQA dataset comprises several question types tailored to evaluate distinct capabilities: MATCH (pattern recognition and relational knowledge), MCQ (topic-based understanding and recall), MCQN (mathematical derivations in a multiple-choice format), and NUM (complex numerical computation and reasoning). The superior performance demonstrated by frontier models on this benchmark substantiates the utility of MaScQA in augmenting LLM capacity for specialized scientific domains.

5.6. Scientific Agents, Foundation Models and Autonomous Laboratories

Researchers analyze the paradigm-shifting role of Large Language Models (LLMs) in fast-tracking the innovation and advancement of nanostructured materials (e.g., MOFs, COFs, and zeolites) in study [81]. Three core applications—NLP text mining, LLM-driven data extraction/science, and autonomous laboratory systems—are used to evaluate the foundations of LLMs and their adaptation (prompt engineering and fine-tuning) (Figure 9). This assessment identifies areas of significant concern regarding prompt engineering versus fine-tuning strategies, as well as the effect of thermal parameters on output consistency, stability, and creativity.

AutoLabs, introduced in [82], is a self-correcting, multi-agent architecture engineered to optimize experimental workflows through self-governing design in chemical research. We perform a methodological assessment of its performance. This model utilizes a multi-agent architecture consisting of a supervisor-orchestrated agent network. This framework leverages automated stoichiometric calculations and self-optimizing mechanisms. This combined architecture achieved the highest accuracy rate (F1-score > 0.89) on complex pathways.

To mitigate the drawbacks of standard LLMs in chemical research, scientists introduce MOFReasoner in [83], a specialized Large Language Model (LLM) fine-tuned to execute scientific queries in chemistry by utilizing Metal-Organic Framework (MOF) adsorption as its foundational concept. This model leverages an extensive data repository—including 8242 research articles and 500 reviews—to retrieve domain-specific data. It demonstrates major improvements in accuracy, reliability, and scientific depth compared to non-specialized models (e.g., GPT-4.5, DeepSeek-R1).

LLEMA [84] (LLM-guided Evolution for MAterials discovery) is a centralized analytical platform architected to navigate the multifaceted decision space in material design. This model combines the generalist scientific intelligence of LLMs with a methodological chemical framework to invent state-of-the-art materials. Through the analysis of LLEMA's capability across 14 industrially critical tasks, the model demonstrates outstanding performance in multi-objective balancing, synthesizability, and memorization.

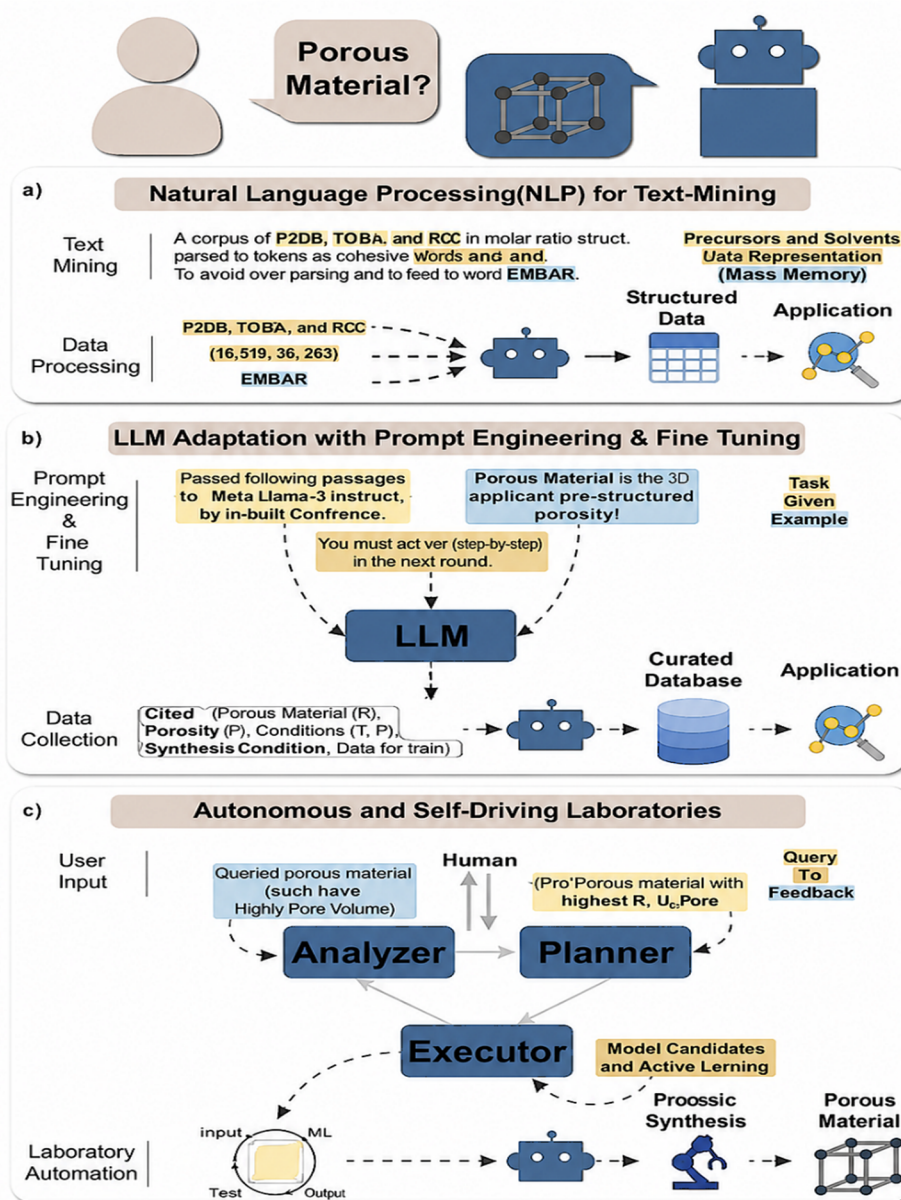


Figure 9. Overall scheme illustrating how language-based methods have evolved within porous materials research [81]: (a) natural language processing (NLP) for text mining of synthesis and property information, (b) the adaptation of LLMs through prompt engineering and fine-tuning to generate structured knowledge, and (c) autonomous systems covering the progression from human-in-the-loop operation to increasingly self-driving laboratory capabilities.

6. Impacts of LLMs in Nanoparticles Research

Large Language Models (LLMs) are emerging as transformative tools in nanoparticle research due to their ability to process large-scale scientific data, accelerate materials discovery and enhance computational decision making.

In nanoscience, researchers often face challenges associated with analyzing vast amount of literature, interpreting multidimensional datasets and optimizing nanoparticle synthesis conditions. LLMs address their limitations by enabling rapid literature mining, automated summarization and intelligent extraction of scientific knowledge from research articles, patents and experimental reports. These capabilities significantly reduce the time required for data collection and hypothesis generation thereby accelerating the pace of innovation in nanoparticle engineering and nanomedicine. Recent advancements in transformer-based AI models have demonstrated strong potential in predicting nanoparticle properties including particle size, stability, toxicity, biocompatibility, catalytic activity and drug-loading efficiency. By integrating multimodal datasets such as spectroscopy, microscopy images, molecular simulations and experimental records LLM assisted systems can identify hidden structure property relationships that are difficult to detect using conventional computational methods.

In biomedical applications, LLMs are increasingly used to support the design of nanoparticle-based drug delivery systems, cancer therapeutics, biosensors and vaccine platforms. AI-assisted frameworks can optimize nanoparticle surface modifications, predict biological interactions and recommend synthesis pathways with improved targeting efficiency and reduced cytotoxicity. Moreover, LLMs contribute to autonomous and high-throughput experimentation by guiding researchers toward optimal experimental conditions and reducing trial-and-error procedures. These improvements not only enhance research productivity but also reduce development costs and resource consumption. Additionally, LLMs facilitate interdisciplinary collaboration by simplifying scientific communication, generating technical reports and supporting multilingual knowledge sharing among global research communities.

Despite these advantages, several challenges limit the unrestricted use of LLMs in nanoparticle research (Figure 10). One major concern is the generation of hallucinated or scientifically inaccurate information, which may lead to misleading interpretations or unsafe experimental outcomes if not carefully validated. Since LLMs rely heavily on existing datasets, biases, incomplete information or low-quality training data may affect the reliability of predictions and recommendations. Ethical concerns regarding data privacy, in, intellectual property, reproducibility and transparency also remain significant particularly in biomedical and industrial nanotechnology applications. Furthermore, although LLMs have immense potential to revolutionize nanoparticle research, their implementation must be accompanied by rigorous experimental validation, human expertise and responsible AI governance to ensure scientific accuracy, safety and reproducibility. Recent studies suggest that the future integration domain-specific LLMs with automated laboratories, digital twins and explainable AI frameworks could further accelerate next-generation nanoparticle discovery and precision nanomedicine development.

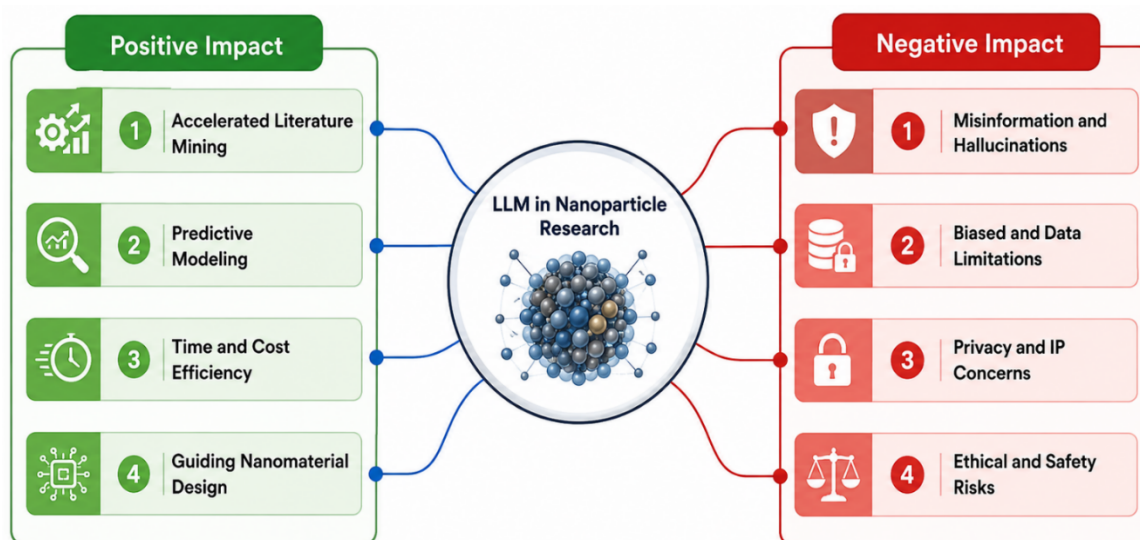


Figure 10. LLM Nanoparticles research impacts.

7. Limitations

Within the domain of molecular and material property prediction, Large Language Models (LLMs) have attained remarkable sophistication, utilizing diverse data formats to project an extensive range of properties [85]. Contemporary research [86–88] indicates that LLMs demonstrate human-level proficiency—and in some instances, superior efficiency—compared to traditional machine learning methods, particularly within limited-resource settings. However, many existing methodologies have only been validated through individual case studies [66]. LLMs have also progressed significantly in the realms of molecular and material design [89–93]. They have proven highly adept across both contexts, especially when refined through specialized, field-specific datasets [94]. Nevertheless, despite this rapid maturation, LLMs exhibit notable deficiencies in pragmatic applications [95]. The high variability of data represents a significant constraint [55], while in nanomaterial discovery, these models encounter issues regarding context-dependent semantic coverage [14].

Furthermore, a paucity of understanding remains regarding nanoparticle interactions across diverse environments [96]. The prohibitive costs of current methodologies and a scarcity of available data continue to impede progression [97]. Additionally, a lack of transparency obscures the reasoning behind model conclusions. There remains a high probability of generating superficially coherent but factually erroneous outputs [79], which is

particularly concerning in safety-critical fields such as medicine. Finally, insufficient training and a systemic reliance on established molecular databases can induce errors and circumscribe accessibility to nascent insights [70].

Despite their growing promise, the use of LLMs in nanoparticle research faces several limitations that must be carefully considered. A major limitation is the quality and availability of domain-specific training data. Nanoparticle research data are often fragmented, heterogeneous, and not always publicly accessible. As a result, LLM outputs may reflect gaps or biases in the underlying literature, which can affect the reliability of predictions and recommendations. Another limitation concerns the limited physical and chemical reasoning capability of current LLMs. Although these models excel at recognizing patterns in text, they do not inherently understand physical laws, thermodynamics, or quantum-scale interactions. Consequently, LLM-generated insights may sometimes lack consistency with fundamental scientific principles unless they are combined with physics-based models or validated through experiments.

The lack of explainability and transparency also remains a key challenge. LLMs often operate as black-box systems, making it difficult for researchers to trace how specific conclusions or suggestions are generated. In scientific research, where interpretability and reproducibility are essential, this opacity can reduce trust and hinder broader adoption. Computational cost and resource requirements represent another practical limitation. Training, fine-tuning, and deploying large-scale LLMs demand significant computational power and energy consumption. This can limit accessibility for smaller research groups and may conflict with sustainability goals unless more efficient model architectures or training strategies are adopted.

8. Future Research Work

The application of LLMs in nanoparticle and nanomaterials research is poised to move from exploratory demonstrations toward deeply integrated production-grade workflows. A near-term priority is the tight coupling of LLMs with experimental automation and simulation platforms to form human-in-the-loop or fully closed-loop discovery systems that can purpose experiments, call simulation tools and interpret outcomes to suggest next steps. Work demonstrating LLMs augmented with domain tools and connected to synthesis platforms shows that agent can plan, call instrument and even assist in robotic execution an important stepping stone toward automated nanoparticle optimization [98].

Another major direction is the development of domain specific, multimodal LLMs that natively ingest and reason over the mix of data typical in nanoscience such as text, spectroscopy and numerical performance metrics. Early multimodal foundation-model work and materials-focused multimodal systems demonstrate improved property prediction and richer reasoning when structural data and text are jointly modeled extending those approaches to nanoparticle morphology, surface chemistry and synthesis protocols should materially improve structure property mapping [99,100].

LLMs can also play a critical role in sustainability, aware nanoparticle design and environmental risk assessment. Reviews and studies show machine-learning tools assisting environmental. Future LLM-based toolchains could help synthesize regulatory texts, aggregate ecotoxicology evidence, suggest safer-by-design modifications and flag likely environmental persistence or biosafety concerns early in the design stage. Integrating environmental assessment modules into LLM workflows will be critical for responsible nanotechnology [101].

In biomedical applications, LLMs and AI-driven models are already influencing nanocarrier design, formulation optimization, and personalized drug-delivery strategies. AI reviews in drug delivery highlight how predictive models, microfluidic integration, and formulation-optimization pipelines can be accelerated by data-driven methods; LLMs can add value by synthesizing literature, generating candidate formulations, and coordinating multi-source data (patient biomarkers, in vitro assays, and nanoparticle descriptors) to propose personalized nanoparticles. Research should focus on integrating LLM suggestions with mechanistic models and clinical constraints for translational impact [102].

9. Closing Remarks

The field of large language models (LLMs) has undergone rapid and transformative growth, leading to unprecedented advances in natural language processing and a wide range of scientific and technological applications. Build upon deep learning networks and the transformative power of the transformer architecture, LLMs have fundamentally changed how machines understand, generate and reason over human language. This review has comprehensive and structured overview of LLMs, covering their historical evolution, core architecture principles, and ecosystem of models and resources that support their development. Furthermore, this work has examined the emerging applications of LLMs across diverse domains, including healthcare, environment, material sciences, and industrial decision-making, highlighting their role in interdisciplinary research, where LLMs facilitate knowledge

integration, accelerate discovery and enhance data-driven insights. In parallel, this review has explored the broader societal implications of LLM adoption, emphasizing their growing influence on scientific workflows, innovation processes, and human-AI collaboration. At the same time, the review critically acknowledges the key challenges associated with LLM deployment, such as data bias, limited transparency, privacy risks, and concerns related to robustness and controllability. Addressing these issues is essential to ensure responsible, trustworthy, and sustainable use of LLMs. As LLM research continues to evolve at a rapid pace, this review serves as a valuable reference for researchers, practitioners and policymakers seeking a holistic understanding of the field.

Author Contributions

M.N.C.E.: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Validation, Visualization, Writing—original draft; J.N.E.: Conceptualization, Methodology, Investigation, Data curation, Formal analysis, Validation, Visualization, Writing—original draft, Writing—review & editing; M.A.A.M.: Project administration; M.M.H.M: Conceptualization, Supervision, Project administration, Validation. All authors have read and agreed to the published version of the manuscript.

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Informed Consent Statement

Not applicable.

Data Availability Statement

No new data were generated in this study.

Conflicts of Interest

The authors declare no conflict of interest.

Use of AI and AI-Assisted Technologies

No AI tools were utilized for this paper.

References

1. Xie, T.; Wan, Y.; Li, W.; et al. Interdisciplinary Discovery of Nanomaterials Based on Convolutional Neural Networks. *arXiv* **2022**, arXiv:2212.02805.
2. Xie, T. Leveraging Large Language Models for Nanomaterials Discovery and Synthesis. Ph.D. Thesis, UNSW Sydney, Sydney, Australia, 2025. <https://doi.org/10.26190/UNSWORKS/30859>.
3. Kim, E.; Huang, K.; Tomala, A.; et al. Machine-learned and codified synthesis parameters of oxide materials. *Sci. Data* **2017**, *4*, 170127. <https://doi.org/10.1038/sdata.2017.127>.
4. Butler, K.T.; Davies, D.W.; Cartwright, H.; et al. Machine learning for molecular and materials science. *Nature* **2018**, *559*, 547–555. <https://doi.org/10.1038/s41586-018-0337-2>.
5. Minaee, S.; Mikolov, T.; Nikzad, N.; et al. Large Language Models: A Survey. *arXiv* **2024**, arXiv:2402.06196.
6. Buehler, M.J. Generative Retrieval-Augmented Ontologic Graph and Multiagent Strategies for Interpretive Large Language Model-Based Materials Design. *ACS Eng. Au* **2024**, *4*, 241–277. <https://doi.org/10.1021/acsengineeringau.3c00058>.
7. Shen, Y.; Zhao, S.; Lv, Y.; et al. Large Language Model-Driven Knowledge Discovery for Designing Advanced Micro/Nano Electrocatalyst Materials. *Comput. Mater. Contin.* **2025**, *84*, 1921–1950. <https://doi.org/10.32604/cmc.2025.067427>.
8. Arya, A.; Garg, D.; Parashar, A.; et al. Nano-AI synergy: Emerging trends, applications, challenges, and future prospects. *Nanotechnology* **2025**, *8*, 100309. <https://doi.org/10.1016/j.nxnano.2025.100309>.
9. Han, S.; Wang, M.; Zhang, J.; et al. A Review of Large Language Models: Fundamental Architectures, Key Technological Evolutions, Interdisciplinary Technologies Integration, Optimization and Compression Techniques, Applications, and Challenges. *Electronics* **2024**, *13*, 5040. <https://doi.org/10.3390/electronics13245040>.
10. Peters, M.E.; Neumann, M.; Iyyer, M.; et al. Deep Contextualized Word Representations. *arXiv* **2018**, arXiv:1802.05365.

11. Mikolov, T.; Chen, K.; Corrado, G.; et al. Efficient Estimation of Word Representations in Vector Space. *arXiv* **2013**, arXiv:1301.3781.
12. Zhang, H.; Yu, P.S.; Zhang, J. A Systematic Survey of Text Summarization: From Statistical Methods to Large Language Models. *arXiv* **2024**, arXiv:2406.11289.
13. Duan, Y.; Zhang, Y.; Yu, R.; et al. Information extraction for materials science using large language models: A survey of recent advances and new frontiers. *Mater. Today Commun.* **2026**, *54*, 115551.
14. Qin, L.; Chen, Q.; Feng, X.; et al. Large language models meet NLP: A survey. *Front. Comput. Sci.* **2026**, *20*, 2011361.
15. Wang, H.; Li, J.; Wu, H.; et al. Pre-Trained Language Models and Their Applications. *Engineering* **2023**, *25*, 51–65. <https://doi.org/10.1016/j.eng.2022.04.024>.
16. Pennington, J.; Socher, R.; Manning, C. Glove: Global Vectors for Word Representation. In Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP), Doha, Qatar, Association for Computational Linguistics, 25–29 October 2014; pp. 1532–1543. <https://doi.org/10.3115/v1/D14-1162>.
17. Vaswani, A.; Shazeer, N.; Parmar, N.; et al. Attention Is All You Need. *arXiv* **2023**, arXiv:1706.03762.
18. Devlin, J.; Chang, M.-W.; Lee, K.; et al. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. *arXiv* **2019**, arXiv:1810.04805.
19. Liu, Y.; Ott, M.; Goyal, N.; et al. RoBERTa: A Robustly Optimized BERT Pretraining Approach. *arXiv* **2019**, arXiv:1907.11692.
20. He, P.; Liu, X.; Gao, J.; et al. DeBERTa: Decoding-enhanced BERT with Disentangled Attention. *arXiv* **2020**, arXiv:2006.03654.
21. Radford, A.; Wu, J.; Child, R.; et al. Language Models are Unsupervised Multitask Learners. *OpenAI Blog* **2019**, *1*, 9.
22. OpenAI; Achiam, J.; Adler, S.; et al. GPT-4 Technical Report. *arXiv* **2024**, arXiv:2303.08774.
23. Touvron, H.; Lavril, T.; Izacard, G.; et al. LLaMA: Open and Efficient Foundation Language Models. *arXiv* **2023**, arXiv:2302.13971.
24. Raffel, C.; Shazeer, N.; Roberts, A.; et al. Exploring the Limits of Transfer Learning with a Unified Text-to-Text Transformer. *arXiv* **2023**, arXiv:1910.10683.
25. Chung, H.W.; Hou, L.; Longpre, S.; et al. Scaling Instruction-Finetuned Language Models *arXiv* **2022**, arXiv:2210.11416.
26. Naveed, H.; Khan, A.U.; Qiu, S.; et al. A Comprehensive Overview of Large Language Models. *arXiv* **2024**, arXiv:2307.06435.
27. Kaplan, J.; McCandlish, S.; Henighan, T.; et al. Scaling Laws for Neural Language Models. *arXiv* **2020**, arXiv:2001.08361.
28. Ouyang, L.; Wu, J.; Jiang, X.; et al. Training language models to follow instructions with human feedback. *arXiv* **2022**, arXiv:2203.02155.
29. Houshy, N.; Giurigu, A.; Jastrzebski, S.; et al. Parameter-Efficient Transfer Learning for NLP. *arXiv* **2019**, arXiv:1902.00751.
30. Hu, E.J.; Shen, Y.; Wallis, P.; et al. LoRA: Low-Rank Adaptation of Large Language Models. *arXiv* **2021**, arXiv:2106.09685.
31. Lester, B.; Al-Rfou, R.; Constant, N. The Power of Scale for Parameter-Efficient Prompt Tuning. In Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing, Online and Punta Cana, Dominican Republic; Association for Computational Linguistics, 7–11 November 2021; pp. 3045–3059. <https://doi.org/10.18653/v1/2021.emnlp-main.243>.
32. Du, N.; Huang, Y.; Dai, A.M.; et al. GLaM: Efficient Scaling of Language Models with Mixture-of-Experts. *arXiv* **2022**, arXiv:2112.06905.
33. Lewis, P.; Perez, E.; Piktus, A.; et al. Retrieval-Augmented Generation for Knowledge-Intensive NLP Tasks. *arXiv* **2021**, arXiv:2005.11401.
34. Sanh, V.; Debut, L.; Chaumond, J.; et al. DistilBERT, a distilled version of BERT: Smaller, faster, cheaper and lighter. *arXiv* **2020**, arXiv:1910.01108.
35. Liu, H.; Li, C.; Wu, Q.; et al. Visual Instruction Tuning. *arXiv* **2023**, arXiv:2304.08485.
36. Wang, A.; Pruksachatkun, Y.; Nangia, N.; et al. SuperGLUE: A Stickier Benchmark for General-Purpose Language Understanding Systems. *arXiv* **2020**, arXiv:1905.00537.
37. Hendrycks, D.; Burns, C.; Basart, S.; et al. Measuring Massive Multitask Language Understanding. *arXiv* **2021**, arXiv:2009.03300.
38. Chen, M.; Tworek, J.; Jun, H.; et al. Evaluating Large Language Models Trained on Code. *arXiv* **2021**, arXiv:2107.03374.
39. Jiang, X.; Wang, W.; Tian, S.; et al. Applications of natural language processing and large language models in materials discovery. *npj Comput. Mater.* **2025**, *11*, 79. <https://doi.org/10.1038/s41524-025-01554-0>.
40. Schilling-Wilhelmi, M. From text to insight: Large language models for chemical data extraction. *Chem. Soc. Rev.* **2025**, *54*, 1125–1150. <https://doi.org/10.1039/D4CS00913D>.

41. Zhao, P.; Zhang, H.; Yu, Q.; et al. Retrieval-Augmented Generation for AI-Generated Content: A Survey. *arXiv* **2024**, arXiv:2402.19473.
42. Singhal, K.; Azizi, S.; Tu, T.; et al. Large language models encode clinical knowledge. *Nature* **2023**, *620*, 172–180. <https://doi.org/10.1038/s41586-023-06291-2>.
43. Hogan, A.; Blomqvist, E.; Cochez, M.; et al. Knowledge Graphs. *ACM Comput. Surv.* **2022**, *54*, 1–37.
44. Ramos, M.C.; Collison, C.J.; White, A.D. A review of large language models and autonomous agents in chemistry. *Chem. Sci.* **2025**, *16*, 2514–2572. <https://doi.org/10.1039/D4SC03921A>.
45. Dastgeer, G.; Shahzad, Z.M.; Chae, H.; et al. Bipolar Junction Transistor Exhibiting Excellent Output Characteristics with a Prompt Response against the Selective Protein. *Adv. Funct. Mater.* **2022**, *32*, 2204781. <https://doi.org/10.1002/adfm.202204781>.
46. Parveen, S.; Misra, R.; Sahoo, S.K. Nanoparticles: A boon to drug delivery, therapeutics, diagnostics and imaging. *Nanomedicine Nanotechnol. Biol. Med.* **2012**, *8*, 147–166. <https://doi.org/10.1016/j.nano.2011.05.016>.
47. Mura, S.; Nicolas, J.; Couvreur, P. Stimuli-responsive nanocarriers for drug delivery. *Nat. Mater.* **2013**, *12*, 991–1003. <https://doi.org/10.1038/nmat3776>.
48. Topol, E.J. High-performance medicine: The convergence of human and artificial intelligence. *Nat. Med.* **2019**, *25*, 44–56. <https://doi.org/10.1038/s41591-018-0300-7>.
49. O'Brien, F.J. Biomaterials & scaffolds for tissue engineering. *Mater. Today* **2011**, *14*, 88–95. [https://doi.org/10.1016/S1369-7021\(11\)70058-X](https://doi.org/10.1016/S1369-7021(11)70058-X).
50. Dagdelen, J.; Dunn, A.; Lee, S.; et al. Structured information extraction from scientific text with large language models. *Nat. Commun.* **2024**, *15*, 1418.
51. Motmans, B. Machine Learning Small Datasets for Cu Nanoparticles: Enhancing Experimental and Computational lab-scale data. Master's Thesis, Hasselt University, Hasselt, Belgium 2025.
52. Pu, Y.; Huang, L.; Lin, T.; et al. Leveraging Large Language Models for Explaining Material Synthesis Mechanisms: The Foundation of Materials Discovery. In Proceedings of the AI for Accelerated Materials Design—NeurIPS 2024, Amherst, MA, USA, 14 December 2024.
53. Dubrovsky, I.; Dmitrenko, A.; Dmitrenko, A.; et al. Unveiling the Potential of AI for Nanomaterial Morphology Prediction. *arXiv* **2024**, arXiv:2406.02591.
54. Lee, S.; Cruse, K.; Gleason, S.P.; et al. Data-driven analysis of text-mined seed-mediated syntheses of gold nanoparticles. *Digit. Discov.* **2025**, *4*, 93–104. <https://doi.org/10.1039/D4DD00158C>.
55. Lee, S.; Cruse, K.; Gleason, S.P.; et al. Data-driven analysis of text-mined seed-mediated growth AuNP syntheses. *ChemRxiv*. **2025**. <https://doi.org/10.26434/chemrxiv-2024-ncjlp>.
56. Sanchez, S.L.; Kim, Y.; Fuhr, A.S.; et al. LLM-Guided Ligand Design for Controlling Nanoscopic Morphology of CsPbBr₃ Perovskite Nanocrystals. *ChemRxiv* **2025**. <https://doi.org/10.26434/chemrxiv-2025-jpp14>.
57. Lv, R. Machine Learning for Controlling the Particle Size Distribution of TiO₂ Nanoparticles in Optical Nanocomposites. *ACS Appl. Nano Mater.* **2025**, *8*, 15323–15335. <https://doi.org/10.1021/acsnano.5c02743>.
58. Abdulai, H. Employing Large Language Models for Systematic Extraction of Nanoparticle Designs from Scientific Literature. Master's Thesis, University of the Balearic Islands, Palma, Spain, 2024.
59. Wang, Y.; Song, H.; Teng, Y.; et al. A Generative Artificial Intelligence Copilot for Biomedical Nanoengineering. *ACS Nano* **2025**, *19*, 19394–19407. <https://doi.org/10.1021/acsnano.5c03454>.
60. Moore, T.L.; Pesce, C.; Greco, A.; et al. Unleashing the Power of Machine Learning in Nanomedicine Formulation Development. *Adv. Funct. Mater.* **2025**, 14387. <https://doi.org/10.1002/adfm.202514387>.
61. Moayedpour, S.; Broadbent, J.; Riahi, S.; et al. Representations of lipid nanoparticles using large language models for transfection efficiency prediction. *Bioinformatics* **2024**, *40*, 342. <https://doi.org/10.1093/bioinformatics/btae342>.
62. Ha, E.; Ha, S.M.; Gerelkhuu, Z.; et al. AI-based nanotoxicity data extraction and prediction of nanotoxicity. *Comput. Struct. Biotechnol. J.* **2025**, *29*, 138–148. <https://doi.org/10.1016/j.csbj.2025.03.052>.
63. Kim, M.; Park, H.; Shin, J. Nanophotonic device design based on large language models: Multilayer and metasurface examples. *Nanophotonics* **2025**, *14*, 1273–1282. <https://doi.org/10.1515/nanoph-2024-0674>.
64. Liu, X.; Sun, P.; Chen, S.; et al. Perovskite-LLM: Knowledge-Enhanced Large Language Models for Perovskite Solar Cell Research. *arXiv* **2025**, arXiv:2502.12669.
65. Peng, C.; Wang, B.; Wu, L.; et al. AI-Driven Discovery and Molecular Engineering Design for Enhancing Interface Stability of Black Phosphorus. *Angew. Chem. Int. Ed.* **2025**, *64*, 202508454. <https://doi.org/10.1002/anie.202508454>.
66. Lin, J.; Zhao, D.; Lu, S.; et al. Conversational Large-Language-Model Artificial Intelligence Agent for Accelerated Synthesis of Metal–Organic Frameworks Catalysts in Olefin Hydrogenation. *ACS Nano* **2025**, *19*, 23840–23858. <https://doi.org/10.1021/acsnano.5c04880>.
67. Marshall, J.; Sanchez, S.; Desai, R.; et al. POLARIS: Perovskite Optimization using LLM-Assisted Refinement and Intelligent Screening. *ChemRxiv* **2025**. <https://doi.org/10.26434/chemrxiv-2025-qqehd-v2>.

68. Faheem, A.B.; Han, Z.; Wu, D.; et al. AI-Driven Big Data Frameworks for Electrode–Electrolyte Interphases in Batteries. *Adv. Mater.* **2026**, *38*, 21975. <https://doi.org/10.1002/adma.202521975>.
69. Zhang, L.; Bing, Q.; Qin, H.; et al. Artificial intelligence for catalyst design and synthesis. *Matter* **2025**, *8*, 102138. <https://doi.org/10.1016/j.matt.2025.102138>.
70. Xian, Z.; Gu, J.; Li, L.; et al. MolRAG: Unlocking the Power of LLMs for Molecular Property Prediction. In Proceedings of the 63rd Annual Meeting of the Association for Computational Linguistics, Vienna, Austria, 27 July–1 August 2025.
71. Zhou, P.; Tim, L.H.; Cheng, Z.; et al. Enhancing Molecular Property Prediction with Knowledge from Large Language Models. *arXiv* **2025**, arXiv:2509.20664.
72. Krotkov, N.A.; Sbytov, D.A.; Chakhoyan, A.A.; et al. Nanostructured Material Design via a Retrieval-Augmented Generation (RAG) Approach: Bridging Laboratory Practice and Scientific Literature. *J. Chem. Inf. Model* **2025**, *65*, 11064–11078. <https://doi.org/10.1021/acs.jcim.5c01897>.
73. Pu, Y.; Huang, L.; Lin, T.; Chen, H.; et al. Leveraging large language models for nano synthesis mechanism explanation: Solid foundations or mere conjectures? *arXiv* **2024**, arXiv:2407.08922.
74. Chandrasekhar, A.; Farimani, O.B.; Ajenifujah, O.T.; et al. NANOGPT: A Query-Driven Large Language Model Retrieval-Augmented Generation System for Nanotechnology Research. *arXiv* **2025**, arXiv:2502.20541.
75. Zhang, B.; Li, Z.; Yang, M.; et al. Initiation performance of spherical LLM-105 with micro-nano structure under short-duration pulses. *Mater. Today Commun.* **2025**, *47*, 113088. <https://doi.org/10.1016/j.mtcomm.2025.113088>.
76. Wang, Yin, X.; Wang, M.; et al. EvoPat: A Multi-LLM-based Patents Summarization and Analysis Agent. *arXiv* **2024**, arXiv:2412.18100.
77. Song, Z.; Zhou, Q.; Ren, C.; et al. LLM-Feynman: Leveraging Large Language Models for Universal Scientific Formula and Knowledge Discovery. *arXiv* **2025**, arXiv:2503.06512.
78. Yin, T.; Feng, R.; Bao, J.; et al. Learning Advance: Robotics-LLM Guided Hypotheses Generation for the Discovery of Chemical Knowledge. *ChemRxiv* **2025**. <https://doi.org/10.26434/chemrxiv-2025-n1b4l>.
79. Su, H.; Chen, R.; Tang, S.; et al. Many Heads Are Better Than One: Improved Scientific Idea Generation by A LLM-Based Multi-Agent System. *arXiv* **2024**, arXiv:2410.09403.
80. Bajjan, C.; Lambard, G. Exploring the expertise of large language models in materials science and metallurgical engineering. *Digit. Discov.* **2025**, *4*, 500–512. <https://doi.org/10.1039/D4DD00319E>.
81. Han, S.; Bae, T.; Kim, J.; et al. Large language models for porous materials: From text mining to autonomous laboratory. *Digit. Discov.* **2026**, *5*, 1470–1500. <https://doi.org/10.1039/D5DD00578G>.
82. Panapitiya, G.; Saldanha, E.; Job, H.; et al. AutoLabs: Cognitive multi-agent systems with self-correction for autonomous chemical experimentation. *Sci. Rep.* **2026**, *16*, 19554. <https://doi.org/10.1038/s41598-026-45593-z>.
83. Bai, X.; Zheng, Z.; Zhang, X.; et al. MOFReasoner: Think like a scientist—A reasoning large language model via knowledge distillation. *Digit. Discov.* **2026**, *5*, 869–877. <https://doi.org/10.1039/D5DD00429B>.
84. Abhyankar, N.; Kabra, S.; Desai, S.; et al. Llama: Evolutionary Search with LLMs for Multi-Objective Materials Discovery. *arXiv* **2026**, arXiv:2510.22503.
85. Zimmermann, Y.; Bazgir, A.; Afzal, Z.; et al. Reflections from the 2024 Large Language Model (LLM) Hackathon for Applications in Materials Science and Chemistry. *arXiv* **2025**, arXiv:2411.15221.
86. Jablonka, K.M.; Schwaller, P.; Ortega-Guerrero, A.; et al. Leveraging large language models for predictive chemistry. *Nat. Mach. Intell.* **2024**, *6*, 161–169. <https://doi.org/10.1038/s42256-023-00788-1>.
87. Qian, C.; Tang, H.; Yang, Z.; et al. Can Large Language Models Empower Molecular Property Prediction? *arXiv* **2023**, arXiv:2307.07443.
88. Jacobs, R.; Polak, M.P.; Schultz, L.E.; et al. Regression with Large Language Models for Materials and Molecular Property Prediction. *arXiv* **2024**, arXiv:2409.06080.
89. Bhattacharya, D.; Cassady, H.J.; Hickner, M.A.; et al. Large Language Models as Molecular Design Engines. *J. Chem. Inf. Model* **2024**, *64*, 7086–7096. <https://doi.org/10.1021/acs.jcim.4c01396>.
90. Liu, G.; Sun, M.; Matusik, W.; et al. Multimodal Large Language Models for Inverse Molecular Design with Retrosynthetic Planning. *arXiv* **2024**, arXiv:2410.04223.
91. Jia, S.; Zhang, C.; Fung, V. LLMatDesign: Autonomous Materials Discovery with Large Language Models. *arXiv* **2024**, arXiv:2406.13163.
92. Jang, H.; Jang, Y.; Kim, J.; et al. Can LLMs Generate Diverse Molecules? Towards Alignment with Structural Diversity. *arXiv* **2025**, arXiv:2410.03138.
93. Lu, J.; Song, Z.; Zhao, Q.; et al. Generative Design of Functional Metal Complexes Utilizing the Internal Knowledge of Large Language Models. *arXiv* **2024**, arXiv:2410.18136.
94. Kristiadi, A.; Strieth-Kalthoff, F.; Skreta, M.; et al. A Sober Look at LLMs for Material Discovery: Are They Actually Good for Bayesian Optimization Over Molecules? *arXiv* **2024**, arXiv:2402.05015.
95. Miret, S.; Krishnan, N.M.A. Are LLMs Ready for Real-World Materials Discovery? *arXiv* **2024**, arXiv:2402.05200.

96. Li, C.; Ma, L.; Xue, Z.; et al. Pushing the Frontiers: Artificial Intelligence (AI)-Guided Programmable Concepts in Binary Self-Assembly of Colloidal Nanoparticles. *Adv. Sci.* **2025**, *12*, 2501000. <https://doi.org/10.1002/advs.202501000>.
97. Krishnamoorthy, U.; Balasubramani, S. Intelligent Nanomaterial Image Characterizations—A Comprehensive Review on AI Techniques that Power the Present and Drive the Future of Nanoscience. *Adv. Theory Simul.* **2024**, *7*, 2400479. <https://doi.org/10.1002/adts.202400479>.
98. Bran, A.M.; Cox, S.; Schilter, O.; Augmenting large language models with chemistry tools. *arXiv* **2023**, arXiv:2304.05376.
99. Tang, Y.; Xu, W.; Cao, J.; et al. MatterChat: A Multi-Modal LLM for Material Science. *arXiv* **2025**, arXiv:2502.13107.
100. Moro, V.; Loh, C.; Dangovski, R.; et al. Multimodal Foundation Models for Material Property Prediction and Discovery. *Newton* **2025**, *1*, 100016. <https://doi.org/10.1016/j.newton.2025.100016>.
101. Scott-Fordsmand, J.J.; Amorim, M.J.B. Using Machine Learning to make nanomaterials sustainable. *Sci. Total Environ.* **2023**, *859*, 160303. <https://doi.org/10.1016/j.scitotenv.2022.160303>.
102. Serrano, D.R.; Luciano, F.C.; Anaya, B.J.; et al. Artificial Intelligence (AI) Applications in Drug Discovery and Drug Delivery: Revolutionizing Personalized Medicine. *Pharmaceutics* **2024**, *16*, 1328. <https://doi.org/10.3390/pharmaceutics16101328>.