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AI for materials

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Today, artificial intelligence (AI) is almost for everything, such as AI for science, AI for life, AI for manufacturing, etc. AI for materials is also a hot topic although the contents are not clearly defined. AI is penetrating into almost every corner of materials science and engineering, i.e, materials discovery and design, materials property prediction, high-throughput materials screening, experiment optimization, autonomous experimentation, modeling of material structure and evolution, and so on.[1]

AI is shocking for its amazing effects of imaging processing, video generation, voice recognition, and text processing. It is surprising that it can accept natural language, i.e., you can type sentences in your mother tongue. Then, the AI model can answer you all kinds of questions, from knowledge to programming, from everyday life questions to professional questions, from values to CIF files (CIF is a file format proposed by the International Union for Crystallography to archive and distribute crystal structure information of materials, including chemical formulas, unit cell parameters, space groups, atomic coordinates, position occupancies, etc.) What AI can do for materials science and engineering? AI models mainly including machining learning models and deep learning models have been widely used as surrogates for quantum mechanics, density functional theory (DFT) and molecular dynamics (MD) to predict the properties of isolated molecules, bulk solids, and materials interface, and for finite element method (FEM) to simulate the physical fields in structures or parts during preparation, fabrication, and service period regardless at the nano-scale or continuum-scale.[2-4] Graph Neural Networks (GNNs) are a new class of machine learning models especially well-suited to the crystal structures and molecules with graph-network representations of atoms (nodes) and bonds (edges) in materials science. Google DeepMind developed graph networks for materials exploration (GNoME) which tweaked the composition of known materials to come up with 2.2 million potential compounds.[5]

What AI can do more? The Large Language Models (LLMs) enable the AI models to communicate with people by natural languages. Beyond that, they can deal with multi-modal inputs, such as image, video, text, voice, etc. The LLMs owns the language reasoning capability, such as understanding and action on natural language instructions, generation of simulation scripts from textual queries, interpretation of scientific visualizations, and forming logical inferences about atomic-level mechanisms. In materials area, the LLMs can reason through user prompts to select suitable materials (e.g., Nb Mo or BCC W), generate accurate LAMMPS input files, and infer the appropriate energy minimization strategies based on simulation goals—mimicking human-like scientific reasoning.[6]

In latest two years, AI gets into AI agent era. An AI agent is a system that autonomously performs tasks by designing workflows with available tools with LLMs as its core. What differentiates AI agents from traditional LLMs is the use of tools and the ability to design a plan of action. The tools available to an agent can include external datasets, web searches and application programming interfaces (APIs). They use the advanced natural language processing techniques of LLMs to comprehend and respond to user inputs step-by-step and determine when to call on external tools.[7] Materials-specific domain knowledge and tools can be integrated with LLMs to form Material AI agents. The domain knowledge can be literatures and references. Recently knowledge graphs are widely used to enhance the domain knowledge representation. For LLM-driven agents can bridge the gap between natural language and domain-specific simulations to accelerate alloy discovery. AI-driven language models—such as BERT, GPT, and their domain-adapted variants like MatBERT and SciBERT—are increasingly capable of extracting, interpreting, and synthesizing this hidden knowledge at scale. LLMs can generalize across different materials by drawing analogies and inferences, relation extraction, and table parsing. LLMs equipped with retrieval-augmented generation (RAG) or hybrid knowledge architectures can access and interpret embedded numerical outputs (e.g., thermal profiles, von Mises stress plots, microstructure evolution maps) across multiple scales.[8]

AI agents incorporate not just software but also hardware tools such as furnace, robots, testing devices. Thus, AI agents may perform the whole process of a discovery of new materials and provide real substance. Autonomous labs (AL) or self-driving labs (SDL) can be established.[9-11] For example, A-Lab, an autonomous laboratory for the solid-state synthesis of inorganic powders. This platform uses computations, historical data from the literature, machine learning (ML) and active learning to plan, drives robotics to do experiments, and interpret the outcomes of experiments. Over 17 days of continuous operation, the A-Lab realized 41 novel compounds from a set of 58 targets including a variety of oxides and phosphates that were identified using large-scale ab initio phase-stability data from the Materials Project and Google DeepMind.[9] Li[12] developed the CARGO system, combining ML and robotics to synthesize horizontally aligned carbon nanotube arrays, test the specimens by Raman spectroscopy, scanning electron microscopy (SEM), and atomic force microscopy (AFM). The obtained carbon nanotube significantly outperformed the traditional catalysts.

The trend of AI agents is multi-agent system or agent of agents with the integration of agents. A multi-agent system (MAS) coordinates multiple artificial intelligence (AI) agents to work collectively to perform tasks.[7] For instance, AtomAgents, a multimodal multiagent AI framework designed to automate the discovery and optimization of metallic alloys with superior mechanical properties. The system leverages a group of specialized AI agents—a planner, coder, image analyst, and simulation agent—each powered by advanced GPT-4-based LLMs and coordinated through the AutoGen framework.[13]

Although AI and LLMs have faced some criticism and questioning, such as hallucinations, poor interpretability, insufficient domain expertise, failure to fully meet user requirements, and high operational costs, etc. But, it should be clarified that the current problem is that the LLMs and LLM agents are undervalued usually because of the users' disappointment and overly optimistic perceptions for AI and LLMs. Fundamentally, the true capabilities and untapped potential of LLMs and agents remain largely underappreciated and unexplored. A key bottleneck lies in the scarcity of interdisciplinary experts who possess both deep AI proficiency and solid domain knowledge in science and engineering fields. Thus, educational reforms are imperative to cultivate a new generation of professionals with integrated expertise in AI, basic science, and applied technology. Only through such interdisciplinary training can we unlock the extraordinary potential of fusing AI with domain-specific knowledge to drive innovation.

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Conflicts of interest

None.

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