MatPilot: an LLM-enabled AI Materials Scientist under the Framework of Human-Machine Collaboration

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1. Introduction

The rapid development of artificial intelligence, especially large language models, provides unprecedented opportunities for materials science research. We have proposed and developed an AI materials scientist named MatPilot, which has shown encouraging capabilities in the discovery of new materials. The core strength of MatPilot lies in its natural language interactive human-machine collaboration, which enhances the research capabilities of human scientist teams through a multi-agent system. MatPilot integrates the unique cognitive abilities, extensive accumulated experience, and ongoing curiosity of humans with the capabilities of AI agents for advanced abstraction, complex knowledge storage, and high-dimensional information processing. It can generate scientific hypotheses and experimental plans, and utilize predictive models and optimization algorithms to drive an automated experimental platform for conducting experiments. Our system has demonstrated remarkable capabilities for efficient validation, continuous learning, and iterative optimization, making it a powerful tool for accelerating the discovery and development of energy storage ceramics.

2. Substantial section

MatPilot consists of a cognition module and a execution module, enhancing materials researchers' ability to think and perform efficiently. The cognition module, analogous to the human brain, is responsible for processing information, analyzing data, and making decisions. Meanwhile, the execution module resembles the body, tasked with performing the practical actions necessary for experimental procedures. Together, these two modules form a cohesive system where thinking and action are interlinked, enabling researchers to conceptualize, strategize, and implement their ideas in practice.

2.1 Cognition module

The cognition module of MatPilot integrates knowledge acquisition and innovation generation as its core functions. The knowledge acquisition function ensures that MatPilot continuously gathers the latest insights in materials science, while the innovation generation function enables it to propose novel research ideas and experimental designs. As shown in Figure 1, this framework presents an innovation generation paradigm built upon multi-agent systems and human-machine collaborative mechanisms. MatPilot can efficiently understand existing research findings and assist in generating new insights, thereby providing substantial support to researchers.

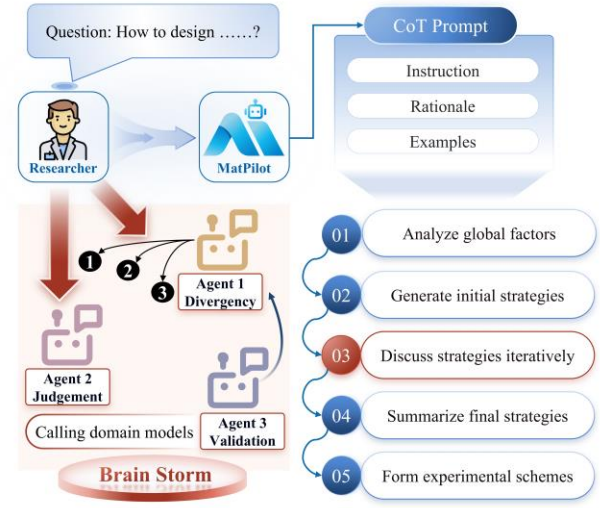

Fig. 1: Multi-agent and human-machine collaboration framework for innovation generation.

2.2 Execution module

The execution module of MatPilot practically implements the research ideas and experimental plans developed by the cognition module. By leveraging automation and autonomous experiments platform, MatPilot's execution module effectively liberates researchers from these tedious experimental tasks, enabling them to devote more time to creative thinking and scientific inquiry. Furthermore, the execution module enhances experimental efficiency through the use of standardized and regulated procedures, thereby significantly improving the reliability and reproducibility of experimental results. Figure 2 shows the automated workstations for energy storage ceramic experiments in the execution module.

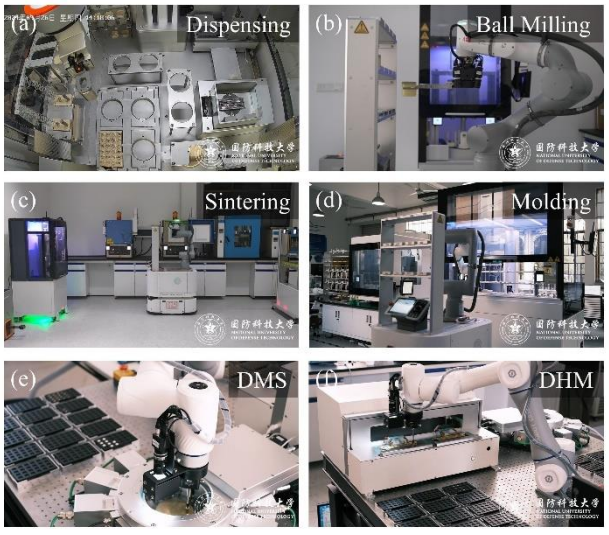

Fig. 2: Automated workstations for energy storage ceramic experiments: (a) Dispensing; (b) Ball Milling; (C) Sintering; (d) Molding; (e) DMS; (f) DHM.