Automating Electron Microscopy for Materials Analysis Using Large Language Model Agents

Dunn, Levi (School: L&amp
N STEM Academy)
Pelaia, Dominick (School: L&amp
N STEM Academy)

Scanning transmission electron microscopy (S/TEM) is essential for atomic-scale research that drives advances in energy materials and nanotechnology, but its operation is limited by labor-intensive expert alignment and rigid automation scripts. This research introduces a novel, generalizable agentic framework for scientific hardware control and research. This architecture integrates a fine-tuned large language model (LLM) with instrument control software, a digital twin simulation environment, and data abstraction layer (DAL) to normalize scientific data into an AI (artificial intelligence)-readable format. Validated on a ThermoFisher Spectra 300 TEM microscope, the framework converts natural-language instructions into executable, multi-device workflows. A dedicated graphical user interface (GUI) facilitates real-time researcher-agent collaboration and allows for the exploration of live spectral and elemental data. Furthermore, our agent renders its plan as a visual, editable workflow that can be reviewed and shared, fostering an open science approach to atomic characterization. The digital twins enable protocol validation before live deployment to ensure safe and reproducible operation. In practice, the system autonomously acquired atomic-resolution images of gold nanoparticles, identified lattice defects, and executed a self-directed fluence experiment to evaluate the material's response to varying electron-beam dosages. This modular architecture provides a blueprint for self-driving laboratories across the physical sciences.

Awards Won:
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