

MAESTRO: An AI agent orchestrator for battery materials discovery

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Modern experimental science is increasingly supported by high-throughput automation, which can execute pre-defined experimental protocols with high precision and repeatability. However, the intellectual core of scientific inquiry (i.e., problem formulation, hypothesis generation, experimental design, result analysis and discussion) remains predominantly human-driven. Therefore, current methodologies can still overlook scientifically meaningful edge cases and alternative experimental pathways [1]. Moreover, as available literature grows at an exponential rate, human researchers are progressively limited in their ability to ask the right research questions and design the next best experimental campaigns.

We present MAESTRO (Materials Acceleration Engine for Synthesis, Testing, and Research Orchestration), a multi-agent AI orchestrator designed to operate in self-driving labs such as DIGIBAT (in Imperial College London) and on materials acceleration platforms such as the FULL-MAP, thereby shifting the focus from mere execution of pre-defined workflows to reasoning-centric design of experiments with minimal human oversight.

To illustrate the extensibility of the framework, we adopt a representative battery design task inspired by Kench et al. [2]: optimising electrode porosity and active-material ratio to maximise cell-level energy density across a range of constant-power discharge conditions (70 W - 190 W). Through a chat interface between a human scientist and the agent (Figure 1), MAESTRO autonomously plans and executes optimisation experiments, and validates predictions as retrieved from a microstructure-to-performance pipeline (i.e., SEM imaging, 2D slice segmentation, SliceGAN reconstruction, TauFactor flow analysis and PyBaMM simulation) [3,4] against experimental results. Additionally, the framework enables the agent to analyse trends from past investigations and draw plausible conclusions for the human scientist.

The preliminary work in MAESTRO offers a conceptual advance in coupling autonomous experimentation with interpretable, innovative scientific discovery. Future work will focus on addressing bottlenecks in scheduling simulation and experimental tasks under time and resource constraints. There will also be an emphasis on benchmarking to evaluate agentic behaviours across laboratories and problem domains.

References

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Figures

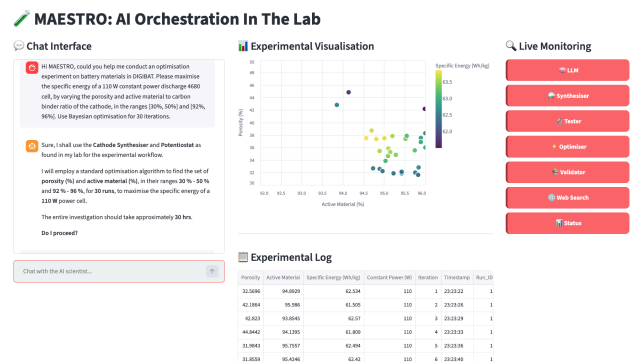


Figure 1. A MAESTRO prototype depicting a chat interaction between a human scientist and an agent, alongside panels for visualising experimental results.