stemOrchestrator: Enabling Seamless Hardware Control and High-Throughput Workflows on Electron Microscopes.

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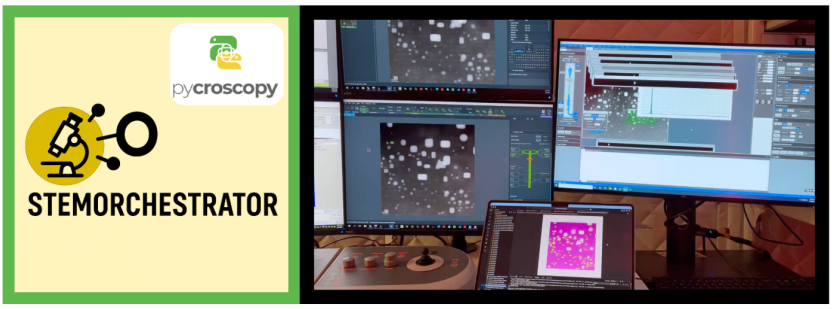

Abstract
Scanning Transmission Electron Microscopy (STEM) is one of the most powerful tools for materials characterization, providing access to atomic-scale structure via direct imaging, chemical composition via spectral methods, and crystallographic information through diffraction. However, these diverse functionalities are often supported by different hardware components from different manufacturers, creating challenges in seamless operation and integration. As the field moves toward machine learning (ML)-enabled experiments and autonomous discovery, the need for coordinated control across these systems becomes critical. Traditional setups lack cohesive automation solutions capable of managing multiple hardware elements and executing complex, adaptive workflows. This paper presents **stemOrchestrator**, a software framework designed to overcome these obstacles by offering a cohesive platform for controlling various STEM hardware modules and developing sophisticated automated workflows. The functionality of **stemOrchestrator**, is demonstrated through its ability to efficiently control multiple hardware components, such as beams, stages, and detectors, and execute intricate workflows like **Particle-mapping** with increased precision and efficiency. Additionally, drift correction integration ensures the reliability of long-term experiments. This research lays the groundwork for a new era in STEM automation, facilitating rapid, reproducible, and collaborative studies in materials characterization. This framework also enables **LLM(Large language model)** agents to potentially intervene, suggest and run complex automated workflows. The codes are available at this link for trying and contributing: https://github.com/pycroscopy/pyAutoMic/tree/main/TEM/stemOrchestrator

I. Introduction

Materials are fundamental to economic development and form the basis for all practical technologies. Over the past twenty years, it has become clear that simply scaling up computational design or synthetic throughput is reaching a bottleneck. Recent advancements in multimodal and high-throughput computational screening and synthesis[1–4] have significantly accelerated the pace of materials discovery. Despite these advancements, a significant bottleneck persists, closing the characterization loop by transitioning from static to dynamic characterization. This transition is crucial for understanding how materials evolve during processing. Electron microscopy and its related spectroscopies provide powerful tools for investigating structural and chemical properties at the single-nanoparticle level[5–7].

Scanning Transmission Electron Microscopy (STEM) is a cornerstone technique in contemporary materials science, renowned for its exceptional imaging, spectroscopy, and diffraction capabilities[8–10]. While artificial intelligence (AI) and machine learning (ML) have demonstrated significant potential to improve microscopy workflows[11–14] the increasing complexity of STEM experiments necessitates advanced automation solutions for efficient hardware integration, data acquisition, and analysis.

Traditional manual or semi-automated methods can be labor-intensive, prone to operator bias, and ill-suited for high-throughput experimentation[12,13]. While recent advancements in AI/ML[15] offer promising possibilities for automation, a **significant challenge** remains the lack of seamless integration and communication among diverse hardware and software components. This obstacle currently hampers the development of sophisticated, fully automated STEM workflows.

Several limitations currently impede efficiency and data quality in STEM operations. Manual control is still primary mode of operation, resulting in operator bias, inaccuracies, and non-reproducibility and inefficiency within workflows. Additionally, a lack of integration among hardware components—often due to non-interoperable APIs—presents significant obstacles to achieving seamless automation. Moreover, long-duration experiments are often compromised by drift in both the sample and microscope alignments, which can affect the ability to collect data and the integrity of that data.

While several systems have been developed to automate specific aspects of Scanning Transmission Electron Microscopy (STEM) workflows, many existing solutions are limited by either their narrow hardware scope or their inability to support complex, multi-modal processes including application's in Cryo-EM where workflows run for days. Pratiush et al. introduced PyAUTOMIC[16,17], a platform designed for automating STEM experiments. However, its control capabilities are primarily restricted to Gatan image filters, limiting compatibility with other hardware. Similarly, Pattison et al. developed Beacon[18] to automate aberration correctors' operations. Although effective in optical alignment and tuning, Beacon does not integrate with spectroscopic detectors like EELS or EDX. Barakati et al. demonstrated the use of custom reward-based segmentation workflows[19] directly on the instrument, but their approach excludes spectroscopic and diffraction acquisition. Cherukara[20] et al. and Welborn[21] et al. have made strides in streaming data analysis for real-time insights during microscopy experiments. However, these systems mainly focus on managing data flow rather than implementing closed-loop instrument control. Several efforts have concentrated on post-acquisition data management and analysis[22–24] but do not integrate with real-time hardware control. Human-in-

the-loop frameworks like hAE[25] support interactive decision-making during microscopy sessions. However, they are limited in their ability to simultaneously query multiple spectroscopic modalities, which restricts their applicability for complex multi-modal workflows. Additionally, active learning approaches using Bayesian optimization have been explored for planning microscopy experiments[26–28]. Despite being effective in theory, many of these methods have only been tested on pre-acquired datasets[29] and lack the real-time hardware interfacing needed for dynamic experimental control.

This work tackles existing limitations in Scanning Transmission Electron Microscopy (STEM) by introducing several key contributions. **First,** it presents the **stemOrchestrator**, a modular software framework designed for unified control over multiple STEM hardware modules, such as the beam and stage, enabling the execution of advanced workflows. **Second**, it introduces Particle-mapping, an exemplary workflow that incorporates AI-driven segmentation to facilitate high-throughput particle characterization within STEM datasets. Lastly, the work integrates a real-time drift correction method to improve experimental stability, ensuring more reliable results during experiments. These contributions collectively enhance both the acquisition and automation capabilities in modern STEM research.

We discuss how the package is designed in section **II** with emphasis on modularity, so it is **easily extensible** as an open-source effort. Section **III** discusses example automated workflow(non-exhaustive) it enables**. Section IV** then talks about the future of integration and development.

II. Design-philosophy

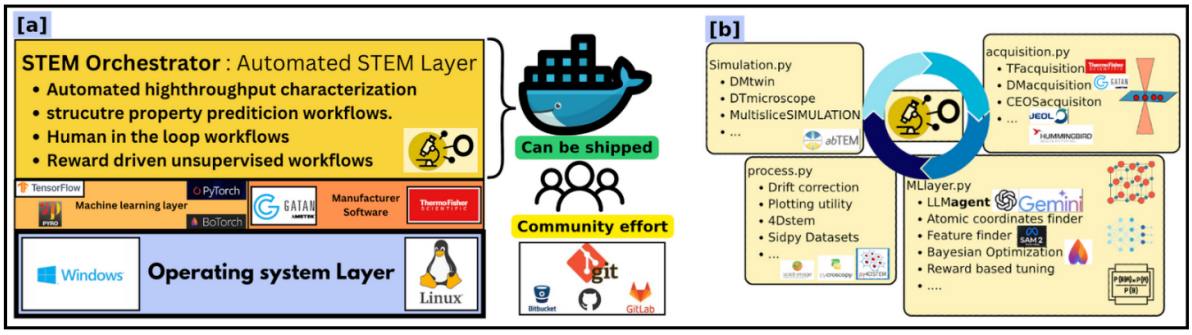

Figure 1. a. shows the stack where stemOrchestraor sits on the software layer. b) shows Visual block layout of stemOrchestrator showing the modularized design philosophy.

The stemOrchestrator, is architected with a modular and cohesive design philosophy, allowing for extensibility, interoperability, and clarity in functionality. The software is organized into four logically separated modules—***acquisition.py***, ***simulation.py***, ***process.py***, ***MLlayer.py*** and ***hardware.py***—each representing a distinct layer of the STEM data pipeline as shown in **Figure 1.**

This structure aligns well with the sequential and interdependent nature of scanning transmission electron microscopy workflows, from data acquisition to ML-guided decision-making. The ***acquisition.py*** module contains multiple acquisition backends such as TFacquisition(Thermofisher STEM controls[30]), DMacquisition(Digitalmicrograph control for eels[16]), and CEOSacquisition(aberration correction control[31]), encapsulating **hardware-specific logic** while exposing a unified interface. This allows the framework to support a

variety of vendor APIs while keeping the orchestration logic decoupled from hardware dependencies. In parallel, the ***simulation.py*** module provides synthetic data generation capabilities by integrating components like DMtwin, DTmicroscope(https://github.com/pycroscopy/DTMicroscope), and Multislice simulation through well-known packages such as abTEM[32] and pyTEMlib(https://github.com/pycroscopy/pyTEMlib). The ***process.py*** module includes essential utilities for processing and visualization, such as drift correction and plotting. The specific hardware level logic is carried out in hardware.py. For example, to CEOSacquisition(aberration correction control[31]) written in ***acquisition.py*** inherits from the lower-level control written in ***hardware.py.***

By isolating this logic into its own layer, the design maintains clarity and reusability across both experimental and simulated datasets. Finally, the ***MLlayer.py*** module is dedicated to advanced machine learning workflows. Tools within this module, including atomic coordinate finders, segmenters based on models like Segment Anything, and large language model api calls, enable intelligent feature detection and reward-based tuning. This layer integrates directly with upstream data while being agnostic to the source, making it suitable for both real and simulated inputs. By structuring the software into interoperable yet functionally specialized components, ensures scalability, ease of debugging, and **future extensibility**—whether adding new instruments, simulations, or ML models. The visual block layout as shown in **Figure 1** of these modules reinforces this design philosophy.

III. Example workflow enabled

In this section, we use stemOrchestrator to illustrate some of the most common workflows, demonstrate their implementation, and propose benchmark examples for evaluating performance and reproducibility.

IIIA. SAM-EDX-EELS-Diffraction

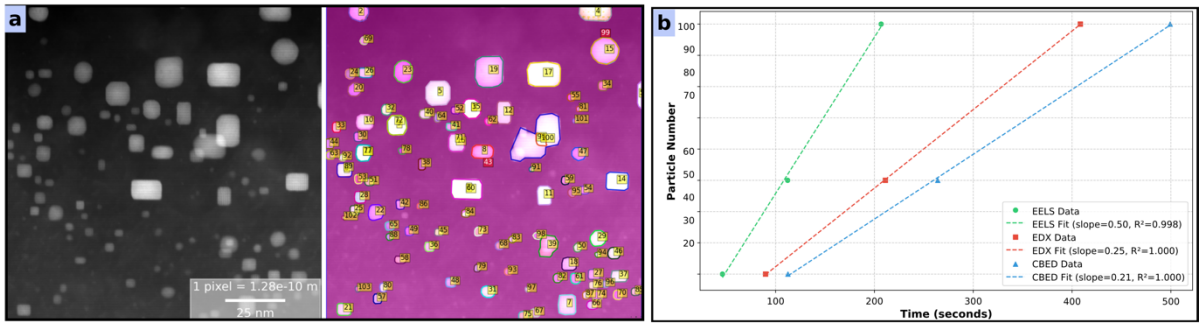

Figure 2. Automated particle analysis using HAADF-STEM imaging and multimodal spectroscopy. (a) Example segmentation maps showing over 100 particles, detected using the Segment Anything Model (SAM). (b) Acquisition times for Electron Energy Loss Spectroscopy (EELS), Energy-Dispersive X-ray Spectroscopy (EDX), and Diffraction across nine experimental runs at different particle counts. The near-linear scaling trend demonstrates the pipeline's efficiency and suitability for high-throughput characterization.

High-throughput particle characterization is a critical need in modern materials research, especially in studies involving heterogeneous nanoparticles and catalytic systems. Traditional Scanning Transmission Electron Microscopy (STEM)-based Electron Energy Loss Spectroscopy (EELS) workflows can take upwards of 10–12 hours to acquire spectrum images for just ~100 particles, often requiring custom scripts to selectively sample only at particle boundaries or centers to reduce overhead.

In this study, we present an accelerated, automated STEM workflow powered by the Segment Anything Model (SAM), enabling rapid, multimodal characterization of particles using Diffraction, Energy-Dispersive X-ray Spectroscopy (EDX), and EELS. As shown in **Figure 2 a**, our pipeline processes datasets with 20+, 50+, and 100+ particles across three magnifications. We demonstrate this capability on a TiO_2–Au sample, where Au nanoparticles are embedded in a TiO_2 matrix. The workflow includes pre-processing to enhance contrast, SAM-based segmentation for robust particle identification, and post-processing to extract morphological and statistical descriptors.

This approach bypasses the bottleneck of manual segmentation and spectrum image acquisition, allowing automated analysis with minimal human intervention. Benchmarking against manually curated datasets confirms that we maintain high accuracy while significantly improving throughput. Specifically, our system acquires EELS data for 100 particles in just ~3 minutes, EDX in ~7 minutes, and CBED Diffraction in ~10 minutes—scaling linearly with particle count, as illustrated in **Figure 2 b**.

The workflow is realized on a ThermoFisher Scientific (TFS) STEM instrument interfaced with the ISAACS supercomputer at the University of Tennessee, Knoxville (UTK). Hardware control and acquisitions (HAADF, EDX, Diffraction) were managed through ThermoFisher AutoScript, while EELS acquisition was automated via the Gatan DigitalMicrograph (DM) Server software using the Gatan Image Filter (GIF). Acquisition times per particle are as low as 0.1 seconds for CBED, 20 milliseconds for EELS, and 2 seconds for EDX. Importantly, this solution is portable and can be deployed on any AutoScript-enabled TFS microscope. Our work bridges deep learning and electron microscopy, providing a scalable, high-throughput solution for rapid characterization of nanomaterials.

III B. Drift correction

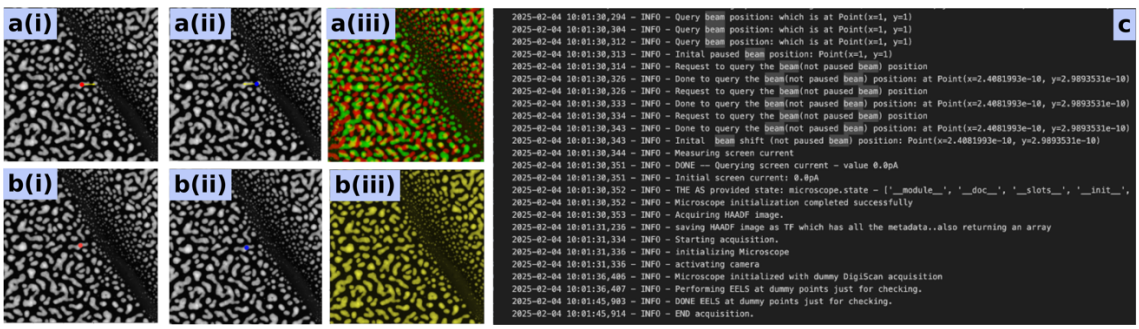

Figure 3. Panels (a) and (b) illustrate an example of the real-time drift correction workflow applied to High-Angle Annular Dark-Field (HAADF) images within the STEM Orchestrator.

In (a), the stage was intentionally shifted to compute drift, resulting in a **measured shift** of 37.14 pixels in X and -0.43 pixels in Y. In (b), **the verification step** shows no drift (Image 1 = Image 2) with a measured shift of 0 pixels in both X and Y. Panel (c) displays an example of the **live logging** output, highlighting how various hardware components are actively queried during the drift correction process.

High-precision microscopy workflows often require dynamic interaction between ML agent and the hardware modules—querying an image, identifying features of interest, determining their coordinates, and then triggering spectroscopic acquisitions at those target locations. However, sample drift during this loop introduces spatial misalignments, which can significantly affect the accuracy of data collection—particularly in tasks requiring nanoscale or even sub-angstrom precision. To address this, we implemented an automated drift correction module within the STEM workflow. Our solution is based on cross-correlation between reference and current images, allowing us to estimate the drift vector and apply the appropriate correction—either by shifting the beam or repositioning the stage. This ensures that subsequent spectroscopic measurements are aligned with the originally selected target points, even if drift has occurred in the interim.

Drift can also be handled using predictive models that learn the underlying behavior of the stage or sample over time, which may be beneficial in high-drift or ultra-precise applications such as atomic-scale manipulation. While these approaches are part of our future roadmap, the current cross-correlation method offers a robust and generalizable solution for most use cases. As shown in Figure 3, this correction module has been integrated seamlessly into the real-time feedback loop of our automated STEM control stack.

III C. Bayesian Optimization and Active Learning for Experimental Automation using Rewards

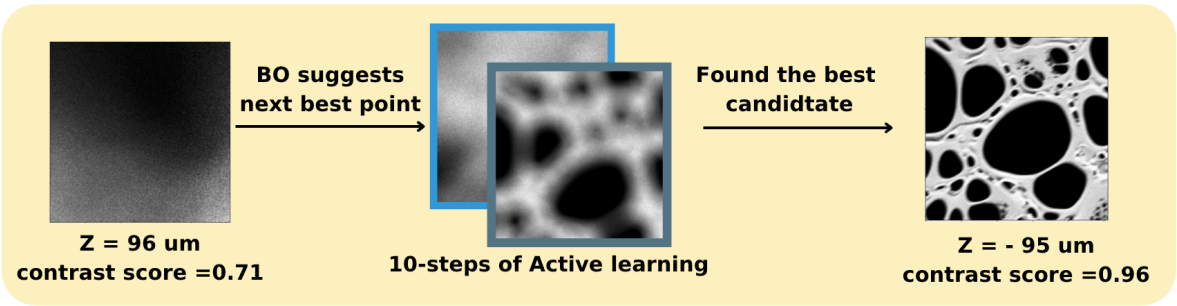

Figure 4. Using BO to tune the sample height of the STEM.

Experimental design in electron microscopy often involves selecting the next measurement point based on prior knowledge, intuition, or visual inspection. However, human decision-making is inherently sequential, potentially biased, and difficult to reproduce. Active learning provides a data-driven alternative by systematically suggesting where to measure next—

balancing exploration and exploitation strategies. This can be formalized as a black-box optimization problem:

$$x^{\cdot} = arg\ \boldsymbol{max}_{x \in X}\ f(\mathbf{x}) \tag{1}$$

where $f(x)$ is an expensive-to-evaluate function (e.g., quality of an image or spectrum), and x represents the experimental parameters (e.g., defocus, aberration coefficients, sample height). Since $f(x)$ is not known a priori and costly to sample, Bayesian Optimization (BO) offers an efficient framework to model it using a surrogate (typically a Gaussian Process, GP) and choose the next point via an acquisition function like Expected Improvement (EI), Upper Confidence Bound (UCB), or Entropy Search.

In microscopy, BO has proven useful in automating parameter tuning tasks. For example:

- BO can help find optimal corrector knob settings that minimize image distortion or maximize image sharpness based on sample height, stigmator coefficients or aberration coefficients values, as demonstrated in prior works like BEACON[18].

- Spectroscopy acquisition (e.g., EELS): BO can guide the microscope to regions with higher likelihood of exhibiting desired features such as elemental peaks, edge plasmons and other desired features in the EELS spectrum[29].

As shown in **figure 4.** The Optimization problem is same as shown in eqn (1), where f(x) is the contrast measure at the different sample height. The sample height "x" can vary for -100 micrometer to +100 micrometer. The contrast measure is defined as

$$f(\mathbf{x}) = \frac{\sigma(\bar{I}(x))}{\mu(\bar{I}(x))} \tag{2}$$

equation 2 defines the objective function, which is being optimized shown in equation 1, $\bar{I}(x)$ is the normalized HAADF image acquired at sample height "x", $\sigma(\bar{I}(x))$ is the calculated std deviation of the normalized image and $\mu(\bar{I}(x))$ is the mean of the normalized image.

Moreover, by leveraging Deep Kernel Learning (DKL), GPs can be made to operate on high-dimensional inputs (e.g., image patches or feature descriptors) enabling richer, context-aware acquisition policies. This integration of BO into real-time feedback loops unlocks new capabilities for adaptive experiments, enabling autonomous optimization of instrument parameters or data quality in a statistically principled and reproducible way.

III. D LLM assisted image understanding and orchestration.

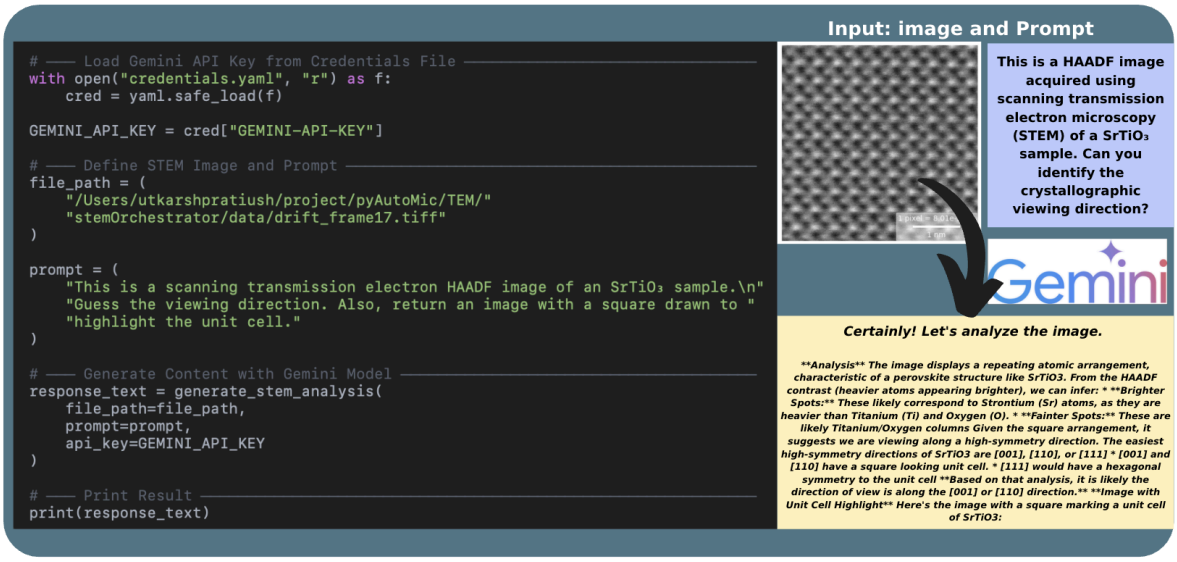

Figure 5. Using LLM in the experimental loop for image understanding.

Large Language Models (LLMs) offer a powerful new interface between microscopy images and actionable experimental insights. **Figure 5** shows an example validating zone axis alignment between literature and acquired image and deciding to tilt the stage to another desired zone axis. Beyond interpretation, LLMs act as **orchestration assistants(to be added in future)**, capable of interfacing across the three layers (Hardware, ML and simulation and experiment logic) of the microscope control stack: Layer 1 (Hardware): LLMs can parse equipment manuals and provide quick guidance on commands, syntax, and expected behavior for hardware-level operations such as stage tilt or beam alignment. Layer 2 (Software & ML): They can recommend analysis workflows, pre-processing techniques, or model selection strategies tailored to the sample and imaging goals. Layer 3 (Experiment Logic): LLMs can suggest adaptive experiment plans, including candidate reward functions for optimization, e.g., maximizing image contrast, minimizing drift, or targeting edge-on interfaces in tomography.

IV. Future work

Building on the modular and extensible design of our current workflow, future efforts will focus on integrating this framework into the broader BlueSky ecosystem[33], enabling real-time feedback loops and multithreaded experimental orchestration in electron microscopy. We also envision **human in the loop** and incorporation of **Large Language Model (LLM)-based agentic workflows**, where intelligent agents can autonomously plan, execute, and adapt microscopy experiments based on literature insights, past data, and predefined scientific goals.

V. Conclusion

In summary, STEM-Orchestrator is a modular, open-source framework that unifies control of diverse STEM hardware, decoupling acquisition, simulation, processing, and ML layers into interoperable modules to enable rapid, high-throughput workflows. We demonstrated its effectiveness through particle mapping an AI-driven segmentation and multimodal spectroscopy pipeline that reduces acquisition times, and a real-time drift-correction module

that maintains nanoscale alignment during extended experiments. By seamlessly integrating Bayesian optimization into live feedback loops. Its cohesive interface to beams, stages, detectors, and existing machine learning and electron microscopy codes not only accelerates materials discovery but also **fosters collaboration and reproducibility** across Machine learning, experiment and simulation communities. The framework's extensible design invites community contributions—whether adding new instrument backends, simulation engines, or advanced AI models—and paves the way for next-generation, LLM-assisted agentic workflows. The source code is available for testing and extension at https://github.com/pycroscopy/pyAutoMic/tree/main/TEM/stemOrchestrator.

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