Final Draft

µStack: An AI-Powered Platform for Atomic Surface Analysis and Microscopy Simulation

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Understanding atomic surface structure is fundamental to advances in catalysis, semiconductor manufacturing, microscopy, fundamental understanding of materials, and more. Current computational approaches require expertise in density functional theory (DFT), management of multiple complex software, and significant computational resources. **µStack (Fig. 1)** is an open-source, AI-driven platform built to address these barriers through a unified interface - simplifying and automating research tasks by combining machine learning potentials (MLIPs), multi-agent workflows leveraging frontier models, and natural language interfaces. The prototype system, built entirely during the hackathon with the aid of AI coding assistants, enables researchers to generate, relax, and analyze atomic surfaces through conversational queries, automatically produce figures, output artifacts (e.g., relaxed structures, simulated microscopy images along with standardized N-Dimensional Spectroscopy and Imaging Data (NSID) data), and summary reports prepared by large language models (LLMs).

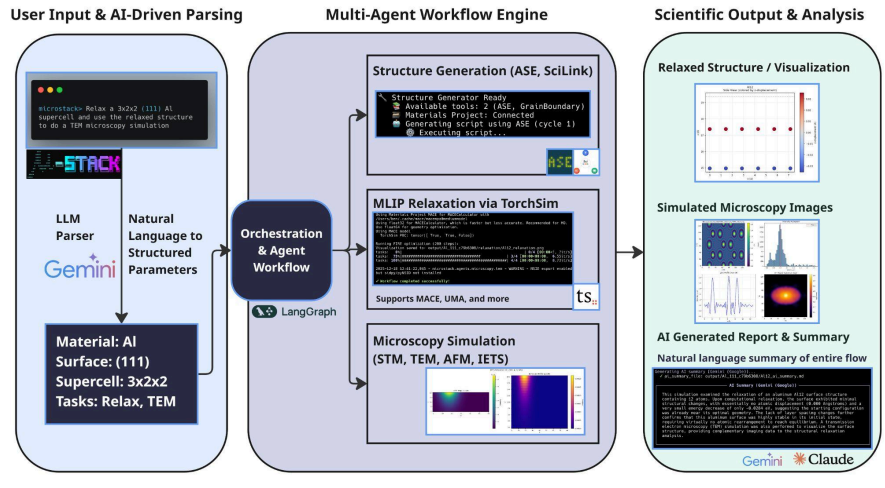

Figure 1: Overview of µStack agent for computational microscopy workflows. The agent converts user queries to tasks and parameters using LLMs (e.g. Gemini). These tasks are passed to the orchestrator to trigger the agent workflow for structure generation, MLIP relaxation, and various microscopy simulations. The outputs are converted into figures along with NSID formatted data, atom positions (xyz files), and a natural language summary.

Methodology

Architecture: µStack employs a multi-agent architecture combining

1. **Query parsing, agent guidance, & orchestration** w/ LLMs (Gemini, Claude) & LangGraph
2. **Structure generation** via the Atomic Simulation Environment (ASE) and SciLink (translates natural language descriptions into valid atomic structures, with sensible defaults)

3. **Atomistic simulation** utilizing modern MLIPs (MACE-MP, UMA via TorchSim) for near-DFT accuracy for relaxation tasks at a fraction of the computational cost
4. **Microscopy simulation:** three modalities including STM via GPAW-based DFT calculations, AFM through the ppafm library with OpenCL acceleration, and Inelastic Electron Tunneling Spectroscopy (IETS) using PPSTM.

Scientific Applications: µStack supports **surface relaxation studies**, allowing researchers to rapidly visualize and predict interlayer spacing changes and **catalysis research**, by simplifying access to simulated surface atomic arrangements for predicting adsorption sites and reaction pathways. Further, the **microscopy simulation** capabilities allow researchers to generate and view predicted STM images, AFM frequency shift maps, and IETS spectra before conducting experiments, enabling hypothesis-driven experimental design. For **2D materials**, the platform supports graphene and transition metal dichalcogenides (MoS2, WS2, MoSe2, WSe2), facilitating research in next-generation electronics and optoelectronics.

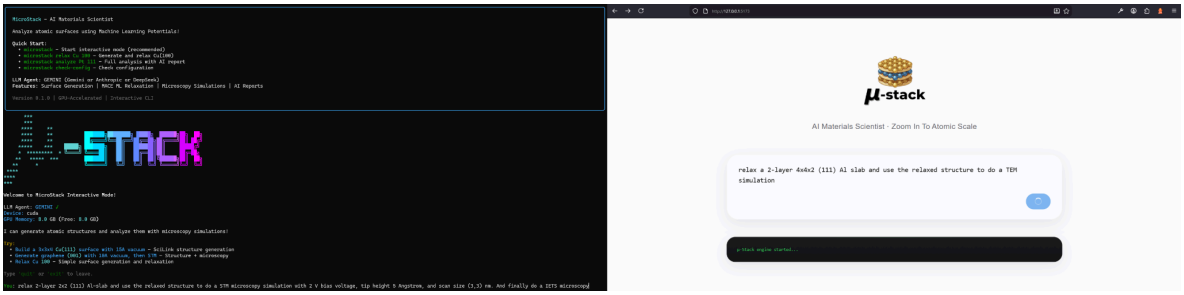

Figure 2: Users can run µStack agent both via (left) interactive terminal and (right) web interface.

User Workflow: A typical µStack session begins with the user providing a natural language query e.g., "Build a 3x3x4 Cu(111) surface with 15 Angstrom vacuum, relax it, then run STM simulation." The LLM-powered parser extracts structured parameters including material composition, supercell dimensions, Miller indices, and requested simulation types. The workflow engine then orchestrates structure generation via SciLink, MACE relaxation using TorchSim, and microscopy simulation in sequence. Upon completion, µStack generates a markdown report containing methodology details, quantitative results, visualization of the relaxed structure, and AI-generated scientific discussion.

Future Directions: In the future, we hope to integrate active learning workflows to enable automated exploration of configuration spaces for identifying promising surface structures for targeted properties. Incorporation of additional MLIPs beyond MACE e.g., CHGNet or M3GNet, would enable ensemble predictions and uncertainty quantification. Real-time integration with experimental microscopy systems could enable on-the-fly comparison between predicted and measured images, accelerating the feedback loop between simulation and experiment. Finally, extension to support adsorbate-surface interactions and reaction pathway modeling would position µStack as a comprehensive platform for computational heterogeneous catalysis, bridging the gap between surface structure prediction and functional materials discovery.

References

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Draft1

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Abstract:

Understanding atomic surface structure is fundamental to advances in catalysis, semiconductor manufacturing, microscopy, fundamental understanding of materials, and more. Current computational approaches require expertise in density functional theory (DFT), management of multiple complex software, and significant computational resources. **µStack (Fig. 1)** is an open-source, AI-driven platform built to address these barriers through a unified interface - simplifying and automating research tasks by combining machine learning potentials (MLIPs), multi-agent workflows leveraging frontier models, and natural language interfaces. The prototype system, built entirely during the hackathon with the aid of AI coding assistants,

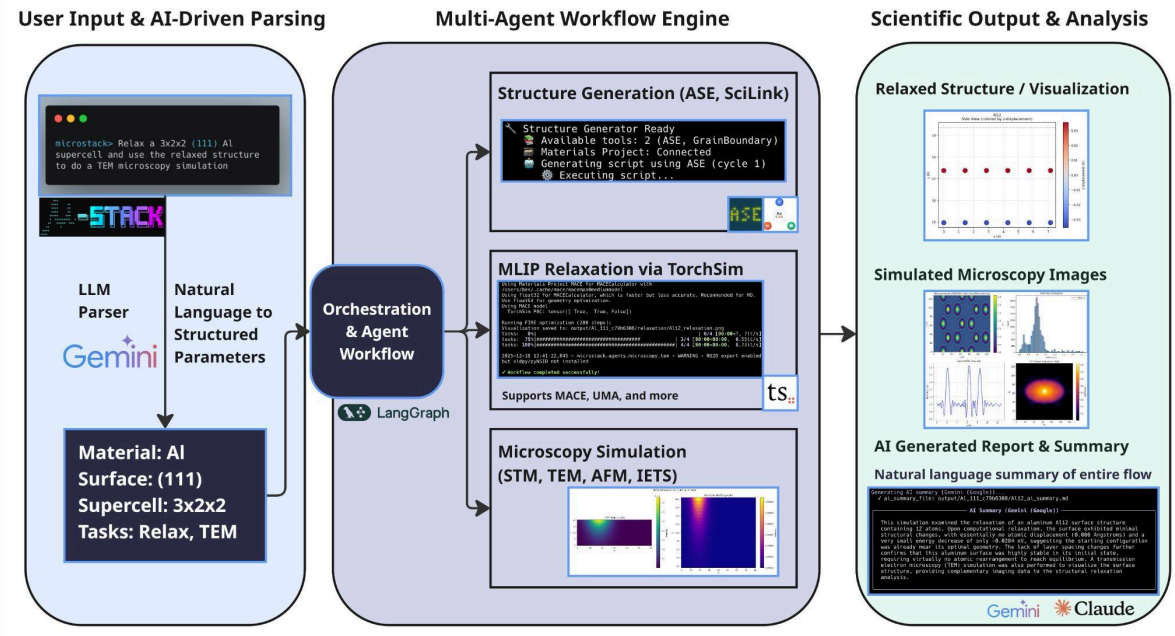

Figure 1: µStack agent to simplify microscopy workflows. The agent converts user queries to tasks and parameters using Gemini (or another LLM of the user's choice). These tasks are passed to the orchestrator to trigger the agent workflow which can access tools including structure generation, MLIP relaxation, and various microscopy simulation. The outputs are then converted into figures along with NSID formatted data, atom positions (xyz files), and a natural language summary.

enables researchers to generate, relax, and analyze atomic surfaces through conversational queries, automatically produce figures, output artifacts (e.g., relaxed structures, simulated microscopy images along with standardized N-Dimensional Spectroscopy and Imaging Data (NSID) data), and summary reports prepared by large language models (LLMs).

Methodology:

Architecture: µStack employs a multi-agent architecture combining modern MLIPs for atomistic simulation, LLMs (e..g, Gemini, Claude) for query parsing and agent guidance, and simulated microscopy orchestrated through LangGraph to enable complex scientific workflows to be executed from simple natural language queries. The **atomistic simulation** utilizes the MACE-MP or UMA MLIPs via TorchSim, providing near-DFT accuracy for relaxation tasks at a fraction of the computational cost. **Structure generation** is powered by the Atomic Simulation Environment (ASE) and SciLink, which translates natural language descriptions into valid atomic structures, using defaults when information is not provided. For **microscopy simulation,** the prototype platform supports three modalities including: STM via GPAW-based DFT calculations, AFM through the ppafm library with OpenCL acceleration, and Inelastic Electron Tunneling Spectroscopy (IETS) using PPSTM.

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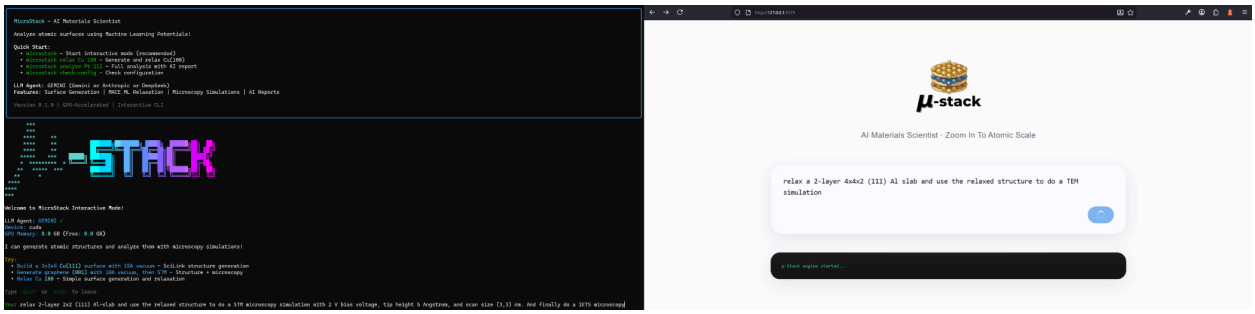

Scientific Applications: µStack is purpose built to address several critical use cases in materials science and microscopy research. µstack supports **surface relaxation studies**, allowing researchers to rapidly visualize and predict interlayer spacing changes and **catalysis research**, by simplifying access to simulated surface atomic arrangements for predicting adsorption sites and reaction pathways. Further, the **microscopy simulation** capabilities allow researchers to generate and view predicted STM images, AFM frequency shift maps, and IETS spectra before conducting experiments, enabling hypothesis-driven experimental design. For **2D materials**, the platform supports graphene and transition metal dichalcogenides (MoS2, WS2, MoSe2, WSe2), facilitating research in next-generation electronics and optoelectronics.

User Workflow: A typical µStack session begins with the user providing a natural language query e.g., "Build a 3x3x4 Cu(111) surface with 15 Angstrom vacuum, relax it, then run STM simulation." The LLM-powered parser extracts structured parameters including material composition, supercell dimensions, Miller indices, and requested simulation types. The workflow engine then orchestrates structure generation via SciLink, MACE relaxation using TorchSim, and microscopy simulation in sequence.

Upon completion, μStack generates a comprehensive markdown report containing methodology details, quantitative results including energy changes and atomic displacements, visualization of the relaxed structure, and AI-generated scientific discussion. The natural language summary provides an accessible interpretation suitable for interdisciplinary collaboration.

Maybe we don't include these for brevity…

Future Directions

Several extensions would significantly expand μStack's capabilities and impact. Integration of active learning workflows could enable automated exploration of configuration space, identifying promising surface structures for targeted properties. Incorporation of additional machine learning potentials beyond MACE, such as CHGNet or M3GNet, would provide ensemble predictions and uncertainty quantification. Real-time integration with experimental microscopy systems could enable on-the-fly comparison between predicted and measured images, accelerating the feedback loop between simulation and experiment. Finally, extension to support adsorbate-surface interactions and reaction pathway modeling would position μStack as a comprehensive platform for computational heterogeneous catalysis, bridging the gap between surface structure prediction and functional materials discovery.

- **Add validation and drawing from experimental data**

Conclusion

MicroStack represents a significant step toward accessible, AI-augmented computational materials science. By combining state-of-the-art machine learning potentials with natural language interfaces and automated report generation, the platform enables researchers to focus on scientific questions rather than technical implementation details, accelerating discovery in surface science and related fields.

References