

Postdoctoral Fellow in AI4Energy

Agentic AI-Guided Discovery in Catalysis and Electrochemical Energy Systems

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SALARY	START DATE	APPOINTMENT	APPLY BY
\$63,480 USD/year	October 1, 2026	12 months (renewable)	September 1, 2026

Ted Sargent and group at Northwestern University invite applications for an accomplished, energetic Postdoctoral Fellow to join AI4Energy, our program building agentic-AI-guided workflows for energy research, with close collaboration opportunities alongside partner teams at Argonne National Laboratory and Lila Sciences.

AI4Energy uses agentic AI — reasoning systems that plan experiments, interpret results in context, and continuously update digital twins — to compress the cycle from hypothesis to validated discovery in catalysis and electrochemistry. Our aim is to develop closed-loop research workflows in which AI models prioritize informative experiments, automated platforms generate high-quality data, and experimental results are used to refine both mechanistic understanding and subsequent decisions. Working alongside Argonne's expertise in catalysis and characterization and Lila Sciences' AI reasoning-and-planning framework, the Fellow will help build closed-loop workflows in which the AI system proposes the most informative next experiment and human researchers supply the mechanistic judgment and hands-on execution that ground it in reality — with the goal of quantifying, concretely, when and how AI-guided workflows accelerate discovery and deepen scientific insights relative to the conventional expert-guided research.

RESPONSIBILITIES

- Design, synthesize, and characterize novel catalysts and electrochemical systems aimed at clean energy conversion and sustainable manufacturing.
- Build and run high-throughput and/or automated electrochemical testing workflows that generate richly labeled, AI-ready datasets linking catalyst synthesis, structure, and performance.
- Partner with Lila Sciences' agentic AI system: review AI-proposed experiments, supply mechanistic feedback, and benchmark AI-guided discovery against expert-guided workflows.
- Collaborate with the Argonne team on complementary characterization and catalytic systems, contributing to a shared, cross-institutional understanding of structure-performance relationships.
- Lead research projects from hypothesis development through first-author publications in high-impact, interdisciplinary journals, and contribute to project milestone reporting and internal research reviews.
- Mentor and advise graduate students and research assistants; contribute to grant writing and the pursuit of external funding opportunities.

QUALIFICATIONS

- Ph.D. in chemistry, chemical engineering, materials science, physics, or a related field, completed or expected before the start date.

- Experience with, and strong interest in, Scientific LLMs; AI/ML-guided or autonomous experimentation (e.g., Bayesian optimization, active learning, Agentic AI); high-throughput experimentation; and scientific programming.
- Hands-on experience designing, synthesizing, and characterizing catalysts or electrochemical systems, with fluency in core experimental techniques such as materials synthesis, device or cell fabrication, and quantitative performance analysis.
- Proficiency with electrochemical and materials characterization techniques, ideally including experience with automated or high-throughput experimental platforms.
- Experience with *in situ* or *operando* characterization techniques for probing catalyst structure, surface intermediates, reaction environments, or degradation mechanisms under working conditions.
- An exceptional, well-documented track record of first-author publications in high-impact, peer-reviewed journals, reflecting independent experimental design, rigorous mechanistic insight, and the ability to carry a research question from hypothesis to publication.
- Demonstrated ability to independently conceive, execute, and troubleshoot research programs, backed by a portfolio of results that reflects technical depth, creativity, and resourcefulness.
- Excellent written and verbal communication skills, and the ability to thrive in a large, multi-institutional, interdisciplinary team spanning Northwestern, Argonne National Laboratory, and Lila Sciences.

HOW TO APPLY

Please include the following in your application package:

- A one-page research proposal responsive to the directions and criteria outlined in this job ad
- Your academic CV, including a section dedicated to your first-authored papers. This should include a list of three referees who are prepared to be consulted

Please use the [application link here](#).