Code: Ref. 26/83

Project: ICREA

Area: Advanced Materials for Energy applications

Group: Nanoionics and Fuel Cells

Group leader: Dr. Albert Tarancón

PI: Albert Tarancón

"R1-PhD Position: Agentic AI for Autonomous Materials Discovery in Next-Generation Energy Devices"

Description:

The Nanoionics and Fuel Cells Group is looking for a passionate MSc graduate to join a transformative PhD project in ***agentic artificial intelligence for accelerated materials discovery***, within the strategic initiative DIREXTE. The research will focus on developing AI agents—built on large language models (LLMs), tool use and multi-agent orchestration—able to reason over scientific knowledge, formulate hypotheses, plan experiments, operate automated laboratory equipment and interpret the results, with the goal of discovering new complex oxide materials for solid-state batteries and solid oxide cells.

The PhD candidate will design, implement and benchmark agentic workflows that combine literature and database mining, machine learning, Bayesian optimization and active learning with closed-loop control of combinatorial synthesis and high-throughput structural and electrochemical characterization. A significant experimental component is an integral part of the project: the candidate will carry out hands-on synthesis and characterization to validate AI-generated hypotheses, generate high-quality data and close the discovery loop between virtual reasoning and real experiments.

This position offers a unique opportunity to work at the frontier between artificial intelligence and materials science, helping to build the scientific tools of the future while contributing to breakthrough advances in electrochemical energy technologies. The candidate will join a vibrant group with strong international collaborations and an ambition to redefine how materials are discovered. We seek a creative, proactive researcher with strong computational skills and a genuine interest in experimental work, excited to contribute to the emerging field of autonomous science.

Qualifications and experience required (at the moment of start):

Essential:

The call is open to candidates of any nationality fulfilling the following criteria:

- Hold a MSc in Physics, Materials Science, Chemistry, Computer Science, Data Science, Engineering or related areas.
- Solid programming skills in Python.
- Fluent in English

Preferred:

- Experience with machine learning and/or large language models (e.g., PyTorch, LLM APIs, agent frameworks such as LangGraph, retrieval-augmented generation, tool calling).
- Knowledge of methods for data-driven experimentation and decision-making (Bayesian optimization, active learning, reinforcement learning).
- Interest in materials science, electrochemistry and solid-state ionics, and willingness to carry out hands-on laboratory work (synthesis and characterization of oxide materials).
- Experience with laboratory automation, instrument control or robotics, and with good software practices (Git, APIs, databases, containers).
- Good communication skills and ability to explain complex scientific ideas to colleagues from different backgrounds.
- Experience in collaborative or interdisciplinary research projects.

Personal Skills:

- Team worker
- Initiative in research and innovation
- Flexibility
- Results-oriented
- Analytical and synthesis capabilities

Required documents:

Applicants must submit the following documents by email to irecjobs@irec.cat and atarancon@irec.cat

Reference:

- Curriculum Vitae, specifying the completed degree and any relevant professional experience.

- BSc and MSc transcripts.

- Motivation letter explaining interest in the project and fit with the position.

Offer of job position:

We offer a **36-month PhD scholarship**
framed within the strategic project DIREXTE. Salaries will follow **IREC's salary policy**, adjusted to the candidate's qualifications and experience.

The **expected starting date** is **December 2026–January 2027**.