

PhD Position Fall 2026 - Montpellier, France

Artificial Intelligence-Driven MOF Materials Discovery for Autonomous Humidity Control

Autonomous humidity control (AHC) systems incorporating advanced porous materials are expected to revolutionize the Ventilation and Air conditioning technologies especially in the context to meet the Green Deal objectives with a climate-neutral economy by 2050. So far none of the conventional porous sorbents/desiccants, such as silica gels and zeolites, are optimal since their moisture adsorption occurs outside the desired RH range and they typically suffer from low adsorption uptake and/or slow adsorption kinetics. Metal-Organic Frameworks (MOFs) have recently been proposed for heat reallocation systems however we are far from fully unlocking the immense potential of this family of materials for water adsorption-based applications since their selection still rely on serendipity. The overall objective of the PhD is to devise **Artificial intelligence (AI)-driven strategy to discover a new generation of MOF water adsorbents with optimal indoor air humidity control performance** by leveraging state-of- the-art **high-throughput (HT) computational screening based on Machine-Learning Interatomic Potentials (MLIP), machine learning (ML) predictive models and AI tools**. This computational work will be performed in strong collaboration with experimentalists expert in HT robot synthesis/characterization and advanced sorption techniques within the priority program France 2030 **PEPR DIADEM AI-MAHC** project (see for more details <https://www.pepr-diaDEM.fr/projet/ai-mahc-2/>). The PhD candidate will benefit from the PEPR DIADEM infrastructure, including advanced platforms, as well as from extensive scientific exchanges enabled by dedicated schools, workshops, and collaborative activities.

Our research group: The successful candidate will join a **strongly connected and international research team** and collaborate with national and international academic partners. Our group is internationally renowned in the field of computational studies of MOFs (see for more information https://scholar.google.com/citations?hl=fr&user=QNfwyjgAAAAJ&view_op=list_works&sortby=pub_date)

Potential candidates: We are looking for a highly motivated Ph.D. candidate with a Master degree or an international equivalent in computer science, physical chemistry, chemical physics, condensed matter physics, statistical physics, theoretical physics, or a related field and a strong interest in materials design. Experience with coding (Python, C, etc.) and force-field- and MILP-based simulations and background in ML/AI tools is an advantage.

Application/ Contact : Interested candidates are requested to submit the following documents to **Prof. Guillaume Maurin**, Institut Charles Gerhardt (UMR CNRS 5253), Université de Montpellier, Institut Universitaire de France, at guillaume.maurin1@umontpellier.fr: **(i)** a curriculum vitae and **(ii)** a motivation letter explaining their interest in the position and how their profile fits the requirements.