PhD: development of physics-based machine learning models for accelerated discovery of spin crossover complexes

A 3-year PhD position is available in Grenoble, France, to work on the development of physics-based machine learning models for the accelerated discovery of novel spin-crossover molecules for a variety of applications. The position is funded by the Multidisciplinary Institute of Artificial Intelligence (https://miai.univ-grenoble-alpes.fr) and **will start before December 2023** under the supervision of Dr Martin Uhrin and Dr Roberta Poloni.

Project summary: Spin crossover occurs in some metal complexes and refers to a change in spin state triggered by an external stimulus such as heat or light. This behaviour is of great interest for applications in spintronics, molecular electronics and sensing. This project will focus on using machine learning coupled with high-throughput electronic structure theory calculations to significantly accelerate the search for candidate materials. You will use uncertainty estimation methods to develop automated, active learning schemes that can learn to accelerate the expensive electronic-structure calculations and help to quickly screen thousands of candidate materials.

Your profile: The ideal candidate will have a master's in physics, chemistry or materials science with experience of atomic scale modelling. Strong programming skills (in e.g. Python, C++, Julia, etc) are highly appreciated as the candidate will be expected to contribute to codes developed within the group that will be disseminated and used in collaborations with groups at Grenoble, EPFL and MIT.

What we offer: A vibrant and highly stimulating environment that is deliberately multidisciplinary in nature, with access to collaborations at both the MIAI and with physicist, chemists and materials scientists at the Materials and Processes Science and Engineering laboratory (SIMAP, https://simap.grenoble-inp.fr) where the candidate will be hosted. The candidate will be supported to become an expert in machine learning methods applied to atomistic systems and electronic structure, highly sought after skills for a future career in academia or industry. They will also have access to an international network of collaborators at MIT, Harvard, EPFL and Microsoft and be encouraged to present their work at international venues.

How to apply: Please send your application **as soon as possible** (detailed CV, motivation letter, and names and contact of at least two references to be joined eventually for recommendation letters) by email to the two supervisors with the subject "MIAI PhD Modelling application". Martin Uhrin (martin.uhrin@epfl.ch) Roberta Poloni (roberta.poloni@grenoble-inp.fr).