Magnetism by machine learning

General Scope : In order to predict new magnetic materials with desired properties on need to be able to scan large number of systems and if possible the whole set of possibilities in a given family of materials. To reach this goal one need to evaluate on-the-fly the magnetic interactions of any given system. The accurate calculation of the latter however presently requires time-consuming procedures. One thus need to change the methodology and use a non-heuristic approach such as machine learning methods. The low computational cost of these new "in silico" methods offers a way to meet the challenge of an "automated" exploration of the field of possibilities.

In the field of magnetic materials, the use of deep learning methods is however quite uncommon and essentially focused on the determination of transition temperature, or phase diagrams and not on the determination of the magnetic interactions.

Research topic and facilities available : In this project, we propose to explore this new field by elaborating a machine learning methodology to predict the magnetic properties of metal-organic-frameworks (MOF). The project will explore the best type of deep learning method to be used, the structural or electronic descriptors needed to predict the magnetic interactions, the construction of the training data sets. The latter will be first developed by collecting data from previous work of the group, then by extending them and producing new data.

This work will be done on French supercomputer facilities. The supervisor will provide the computer hours allocation.

Possible collaboration and networking : This work will be done in close collaboration with a machine learning speciatlist :Jean-Luc Parouty from SIMAP. The student will also be in contact with other theoreticians specialist of evolutionary algorithms (Gilles Frapper and F. Guégan from IC2MP) or neutrons scattering (Elisa Rebolini from ILL) and experimentalists groups working on magnetic MOFs.

Possible extension as a PhD : yes

Required skills: A good knowledge of quantum mechanics is required as well as basic knowledge of python and linux operating system. Some knowledge on machine learning and magnetism will be appraciated.

Starting date : Anytime between february and april 2023

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