

Machine learning for magnetism

General Scope : Machine learning methods are new tools whose possibilities researchers are intensively exploring for new scientific domains over the last 2-3 years.

The knowledge of complex magnetic orders is one of the key point in the domain of multiferroics (systems in which magnetic and electric degrees of freedom are coupled) or spintronics. Indeed the manipulation of such orders is one of the challenges for tomorrow computers (low-energy memories, sensors, 4-bits logic, etc.). Those complex orders are however difficult to decipher as one not only needs the knowledge of precise effective magnetic interactions, but also the way they induce long range order.

Research topic and facilities available : Machine learning methods have proven very efficient for the determination of phases diagrams, and long-range orders generated from sets of magnetic effective interactions. However the knowledge of the set of magnetic interactions for a give compound still remains a difficult, time-consuming, task.

The main objective of this internship will be to explore the possibility to predict magnetic interactions using deep learning methods.

This is a theoretical subject aiming at exploring the possibilities offered by a new domain. The student will thus have to learn deep learning methods, but also the physics underlying the effective magnetic interactions in a material and the ab-initio methods able to accurately evaluate them (a package have been recently developed for this purpose in our group). The student will be using national and/or regional supercomputer centers during this internship.

Possible collaboration and networking :

The student should work with our collaborators in DL (from SIMAP, Grenoble), in magnetism and ab-initio calculations (from ILL), as well as quantum chemists from Poitiers University and experimental chemists from Lyon whether this internship will foster a PhD.

Possible extension as a PhD : yes

Required skills: master in Physics, Quantum Chemistry or Computer Science (if the student has a good knowledge of deep learning methods). The knowledges needed for this internship are Quantum Mechanics, Machine Learning and the usage of linux computers. As this is a interdisciplinary spectrum, the student will have to learn during the internship the part of these domains she/he is not presently familiar with.

Starting date : anytime in the first part of 2022

Contact :

Name : LEPETIT Marie-Bernadette

Institut Néel - CNRS

Phone : 04.76.88.90.4

e-mail : Marie-Bernadette.Lepetit@neel.cnrs.fr

More information : <http://neel.cnrs.fr>