PhD funding in machine learning applied to the inorganic chemistry

Candidates should send their CV and Master Degree details transcript at

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** before the 21th September**

Data-driven materials discovery is appearing as an immense boom. In such a paradigm, computational models trained to find new patterns in massive chemical datasets will rapidly scan compositions and systematically identify attractive candidates for technological applications.

In the present thesis, the PhD candidate will challenge the problem of discovering new crystal structures by applying modern machine learning (ML) approaches to design new and efficient materials for energy.

The study will be applied to materials useful for energy storage, such as metal hydrides able to store safely and reversibly large amounts of hydrogen. The proposed original approach results from the complementarity of interdisciplinary groups in both chemistry (ICMPE-Thiais) and statistical machine learning (Sorbonne université, Paris). First, a learning database will be built where the descriptors are physical properties (like enthalpy obtained from massive DFT calculations). Then, we propose not only to apply the state-of-the-art statistical methods, as neural networks, but also to develop novel algorithms (as generative GAN) specific to materials science applications.