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SEMINAIRE

Lundi 14 juin 2021 à 10h – Visioconférence

Gian-Marco Rignanèse

Research Director of the Fund for Scientific Research (F.R.S.-FNRS Belgium)
« Professeur extraordinaire », Ecole Polytechnique de Louvain - Belgique

«Materials informatics: the combined power of high-throughput ab initio calculations and machine learning»

The last decades have witnessed a considerable progress in the capabilities of ab initio simulation codes. Combining these developments with the increase in the supercomputing power, it has become possible to screen thousands of materials searching for specific simple properties. In this talk, I will first briefly present this so-called high-throughput ab initio approach and its most recent achievements. For more complex properties, this high-throughput ab initio approach is still out of reach because of the required CPU time. To overcome this limitation, artificial intelligence has recently attracted much attention. However, in order to make accurate predictions, current machine-learning approaches generally require large amounts of data, which are precisely not available for complex properties. Therefore, I will introduce the MODNet framework which relies on a feedforward neural network and the selection of physically meaningful features. Next to being faster in terms of training time, this approach is shown to outperform current machine-learning models on small datasets. Finally, I will illustrate the combined power of high-throughput ab initio calculations and machine learning through a few recent examples.

Contact : Cyril Aymonier (DR CNRS, ICMCB)

Short bio

G.-M. Rignanese received his Engineering degree from the Université catholique de Louvain in 1994 and Ph.D. in Applied Sciences from the Université catholique de Louvain in 1998. During his Ph.D., he also worked as a Software Development Consultant for the PATP (Parallel Application Technology Project), collaboration between CRAY RESEARCH and Ecole Polytechnique Fédérale de Lausanne (EPFL) in the group of Prof. Roberto Car. He carried his postdoctoral research at the University of California at Berkeley in the group of Prof. Steven Louie. In 2003, he obtained a permanent position at the Université catholique de Louvain.

He is especially active in high-throughput approaches collaborating to the Materials Project. He is also part of the OPTIMADE consortium which aims to work in the direction of making materials databases interoperational by developing a common REST API. More recently, he also started exploiting machine learning to predict the properties of materials. Furthermore, his group plays an active role in the development of different softwares (Abinit, Abipy, PyMatGen,FireWorks) and pseudopotentials through the PseudoDojo. In 2019, he was named APS Fellow for original efforts developing free license software in the field of electronic structure calculations, and high-throughput calculations in a broad range of materials types.