# Master 2: *International Centre for Fundamental Physics*
INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
CNRS   identification code: IMPMC – Sorbonne University
Internship director'surname: A. Marco SAITTA – PR Classe Exceptionnelle
e-mail: marco.saitta@sorbonne-universite.fr   Phone number: 0144272244
Internship codirector'surname: Fabio PIETRUCCI – IMPMC (SU)
Internship location: IMPMC – SU – Campus Pierre et Marie Curie
Thesis possibility after internship: YES
Funding: Very likely (Labex/Idex), or ED's   If   YES, which type of funding:

Machine learning methods for polymorphism and critical phenomena in exotic liquids

First-order phase transitions are common in the solid state but for a long time judged incompatible with the nature of the liquid state. About 20 years ago, such a liquid-liquid transition (LLT) was discovered in elemental phosphorus, which has had a large impact in the scientific community as it
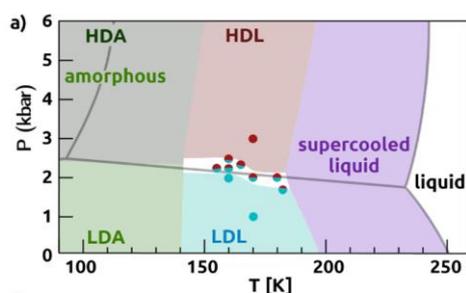
changed the way the liquid state was perceived. Since then, no other example of a LLT separating two thermodynamically stable liquid phases of a pure substance could be experimentally evidenced, until a recent experimental discovery of a LLT in compressed liquid sulfur by colleagues in our team [Nature (2020)]. We have recently proved, by theoretical calculations, that water, instead, does not exhibit a LLT [PNAS, under review, see figure], ending a 30-year long debate in the community.

Building on our recent experimental and theoretical breakthroughs, achieved thanks to state-of-the-art free-energy methods, we are strengthening our approaches through the in-house ongoing development of quantum accuracy-level machine learning potentials, capable to address challenges in the study of chemical reactions in more and more complex and realistic environments. In this internship project, which will lead to a PhD thesis, we will develop a machine learning (ML) description of liquid sulfur, trained on ab initio simulations; the ML description will allow us to explore the sulfur phase diagram (both in its liquid and solid phases) at an unprecedented level of both accuracy and complexity.

We look for a student willing to develop these innovative methods and determined to carry out the project in connection with our network of collaborations. We have a consolidated expertise and a strong publication record including, in the last few years, 7 PNAS, 5 PRL, 4 SciRep, 2 Nature Comm, 1 Nature Methods.

Techniques/methods in use: statistical analysis, clustering, inference, local and global descriptors, ab initio molecular dynamics

Applicant skills: strong background in statistical physics, interest in computational methods, knowledge on transformations in condensed matter.

Key words: theory, statistical mechanics, simulations, machine learning

The team (scan the codes, see what we look like "in action"):

A. Marco Saitta, Full Sorbonne U Professor of Physics, team leader

Video from my General Seminar at the Physics Department of ENS

Fabio Pietrucci, Assistant Professor SU of Physics at IMPMC, expert of Advanced Statistical Mechanics and Thermodynamics methods

Video snippet from my course at the Paris International School on Advanced Computational Materials Science

Condensed Matter Physics: YES	Macroscopic Physics and complexity: YES
Quantum Physics: YES	Theoretical Physics: YES