SCIENCES SORBONNE UNIVERSITÉ

2021-2022

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

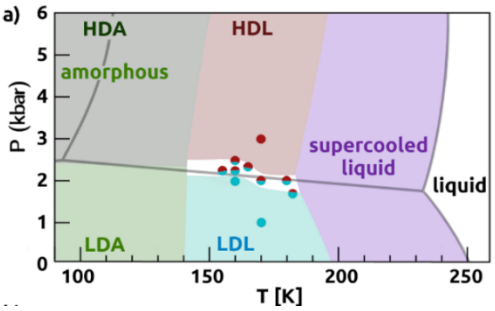
Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: A. Marco Saitta

Title: Polymorphism and critical phenomena in liquid sulfur studied by machine learning methods

Keywords: Liquid-liquid transition, critical phenomena, ab initio simulations, machine learning, phase space explorations

Scientific description:

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 one of us [L. Henry et al, Nature 584 (2020)]. We have recently proved, by theoretical calculations, that water, instead, does not exhibit a LLT [PRX, 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 undertake these innovative methods and determined to carry out this project within a strong collaboration between theory and experiments. We have a consolidated expertise and a strong publication record including in the last few years, in the theoretical part only, 8 PNAS, 5 PRL, 4 SciRep, 4 J. Phys. Chem. Lett. 2 Nature Comm, 2 Phys Life Rev, 1 Nature Methods, 1 ChemSci.

Techniques/methods in use: statistical analysis, *ab initio* molecular dynamics and free-energy methods, machine learning

Applicant skills: strong background in statistical physics, interest in computational materials science, basic knowledge in transformations in condensed matter physics and chemistry

Industrial partnership: N

Internship supervisor(s) (name, email, phone, webmail):

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Internship location: IMPMC – Campus Pierre et Marie Curie – T 2324

Possibility for a Doctoral thesis: Y (specific funding very likely, otherwise doctoral school)