

Internship offered in M2 2018-2019

Responsible for internship

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Internship topic: Unveiling the nature of hydrides high-temperature superconductors

The sulfur hydride H_3S is the highest-temperature superconductor known so far. It superconducts up to 205 K at 15 GPa. It has been discovered a few years ago, thanks to the development of diamond anvil cells with in situ conductivity measurements. It is supposed to be a phonon-driven BCS superconductor. While density functional theory (DFT) suggests that the record-breaking superconducting temperature takes place at pressures in proximity the phase transition between the Im-3m and the lower-pressure R3m phase, the transition pressure does not match the experimental results, questioning the validity of the DFT picture.

By using advanced quantum Monte Carlo techniques, known to be very accurate, we plan to study the structural phase responsible for the astonishing high superconducting temperature in this class of materials. The outcome of this work will be fundamental to understand its electronic properties and their interplay with its crystal structure, very hard to access experimentally for the light atomic number of H and for the extremely high-pressure conditions. Therefore, our theory contribution will be invaluable to shed light on the nature of these breakthrough materials.

Techniques involved: Density functional theory, quantum Monte Carlo

Paid internship: Yes

Can this internship be continued for a PhD? Yes

If yes, type of PhD funding envisaged is: Bourse du Ministère