2020-2021

Master thesis proposal

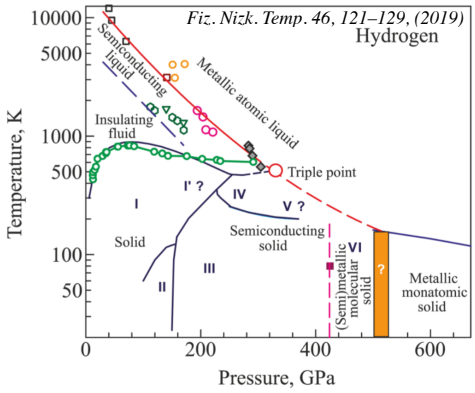
Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: Guillaume Fiquet

Title: *Electron correlation in high-pressure solid hydrogen phases*

Keywords: ab initio simulations, electronic structure, phase transitions, many-body theory, density functional theory (DFT)

Scientific description:
Hydrogen is naturally found in molecular compounds but solidifies in its pure form in high-pressure environments such as the interior of planets. So far, we have a very limited knowledge of its crystal structure as hydrogen is elusive, posing a challenge to experiments. Therefore, theory predictions are fundamental to explain the hydrogen phase diagram. At low temperature, it is known to contain several stable molecular solid phases that at sufficiently high pressure dissociate into a metallic atomic solid with exotic properties due to strong electron-electron and electron-lattice interactions. This project aims to identify the drawbacks of standard DFT methods for treating many-electron effects in solid hydrogen and to study how these can be overcome by applying more advanced Green's function techniques that systematically include electronic correlation. We then aim to predict the relative energies between various high-pressure phases and study their metal-insulator transitions, which could lead to high-temperature superconductivity.



Techniques/methods in use: Many-body theory (DFT and beyond), Electronic structure codes (Quantum Espresso)
Applicant skills: Background in solid-state or chemical physics. Strong interest in theory and simulations. Basic programming skills.
Industrial partnership: No

Internship supervisor(s):
Maria Hellgren, Michele Casula
E-mail: maria.hellgren@upmc.fr, Tel: 01 44 27 52 23
Internship location: Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC), Equipe: TQM: http://www.impmc.upmc.fr/fr/equipes/theorie_quantique_des_materiaux.html,
Possibility for a Doctoral thesis: Yes