2019-2020

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: *Design of high pressure carbides with extended carbon frameworks*

Keywords: Carbon, high pressure, materials design

Scientific description:

The main objective of this project is to explore new carbon compounds using high pressure as a stabilization tool for newly theoretically predicted "polymerized" anionic carbon states. For example 3-D clathrate superstructures are expected to have mechanical properties comparable to diamond, typical dielectric and highly covalent compound, and at the same time be metallic and even superconductors as some silicon clathrate analogs. Other phases are expected to be semiconductors with direct bandgap in visible domain, i.e. very promising materials for optoelectronics.

In the framework of current traineeship, we propose to study phase transformations and chemical interactions in a number of Carbon-Metal systems with promising precursors at high pressure-temperature conditions using "large volume" high-pressure synthesis techniques. The research will be focused on the search of new advanced materials, their recovery and characterization at ambient conditions.

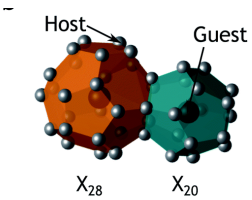

Figure. *Here is one of expected crystal structure, produced by rigid covalent framework of carbon atoms (hosts) with intercalated metal atoms (guests). Simultaneous coexistence of covalent and metallic bonds is expected to give rise to a unique combination of physical and chemical properties: extreme hardness comparable to diamond, lightness (low density), metallic electrical and thermal conductivity, superconductivity.*

Techniques/methods in use: **High pressure techniques, PPMS, NMR, X-ray diffraction**
Applicant skills:
Industrial partnership: No

Internship supervisor(s) : Alexandre Courac (alexandre.courac@upmc.fr)
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Internship location: IMPMC, 4 place Jussieu, 75005 Paris

Possibility for a Doctoral thesis: Yes