

PhD subject: Alkaline silicides and germanides for energy applications

Keywords: Energy, High-Pressure High-Temperature, Neutron diffusion and diffraction

Abstract: This project is motivated by the high toxicity, high cost and / or scarcity of the elements currently used in the field of energy, in particular for the storage of energy in batteries and for the conversion of the heat lost in electricity in the thermoelectric modules. The goal is to develop and study new environmentally friendly alkali silicides for energy applications.

In this context, our research strategy will combine DFT calculations (Stability, Electronic Structure, Lattice dynamics), non-equilibrium syntheses (High-Pressure High-Temperatures) and large-scale facilities characterizations (elastic, quasi-elastic, inelastic diffusion of neutrons). We will focus on complex structures such as open networks (tunnels, interconnected cages) favorable to the diffusion of alkaline atoms for energy storage applications. Among them, some are semiconductors and are expected to have a low thermal conductivity due to their structural complexity, finding here an interest in applications related to thermoelectricity.

The objectives of this project follow these guidelines and will be:

- to synthesize new metastable alkaline silicides and germanides under High-Pressure High-Temperature,
- to characterize the sample (DRX *in situ*, SEM, EDS, HR TEM, neutron diffraction),
- to study the lattice dynamics by combining vibrational spectroscopies (IR, Raman, inelastic neutron scattering) and *ab-initio* calculation,
- to study the diffusion mechanisms in open framework with quasi-elastic neutron scattering
- to characterize the electrochemical properties (in Li-ion batteries) and the thermoelectric properties of the most promising compounds.

Candidate profile: The candidate should have a background in materials science, physics or solid-state physics and chemistry and a strong motivation for experiments. French language is not required and will be improved in the laboratory. However, fluent English (spoken, read, written) is mandatory for foreign candidates.

Location: The work is part of a cooperation between Montpellier, Grenoble and Paris. It will be held at the Institute Charles Gerhardt Montpellier (ICGM - Montpellier) with chemists, physicists and metallurgists for one year and at the Institute Laue Langevin (ILL - Grenoble) for two years. The candidate will also visit several times IMPMC (Paris) during his PhD.

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